Second-order Gauge-invariant Cosmological Perturbation Theory: Current Status

Kouji Nakamura
Optical and Infrared Astronomy Division, National Astronomical Observatory of Japan, Osawa, Mitaka, Tokyo 181-8588, Japan.

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The current status of the recent developments of the second-order gauge-invariant cosmological perturbation theory is reviewed. To show the essence of this perturbation theory, we concentrate only on the universe filled with a single scalar field. Through this review, we point out the problems which should be clarified for the further theoretical sophistication of this perturbation theory. We also expect that this theoretical sophistication will be also useful to discuss the theoretical predictions of Non-Gaussianity in CMB and comparison with observations.

I. INTRODUCTION

The general relativistic cosmological *linear* perturbation theory has been developed to a high degree of sophistication during the last 30 years[1–3]. One of the motivations of this development was to clarify the relation between the scenarios of the early universe and cosmological data, such as the cosmic microwave background (CMB) anisotropies. Recently, the first-order approximation of our universe from a homogeneous isotropic one was revealed through the observation of the CMB by the Wilkinson Microwave Anisotropy Probe (WMAP)[4, 5], the cosmological parameters are accurately measured, we have obtained the standard cosmological model, and the so-called "precision cosmology" has begun. These developments in observations were also supported by the theoretical sophistication of the linear order cosmological perturbation theory.

The observational results of CMB also suggest that the fluctuations of our universe are adiabatic and Gaussian at least in the first-order approximation. We are now on the stage to discuss the deviation from this first-order approximation from the observational[5] and theoretical sides[6, 7] through the non-Gaussianity, the non-adiabaticity, and so on. These will be goals of future satellite missions. With the increase of precision of the CMB data, the study of relativistic cosmological perturbations beyond linear order is a topical subject. The *second-order* cosmological perturbation theory is one of such perturbation theories beyond linear order.

Although the second-order perturbation theory in general relativity is an old topic, a general framework of the gauge-invariant formulation of the general relativistic second-order perturbation has been proposed[8, 9]. This general formulation is an extension of the works of Bruni et al.[10] and has also been applied to cosmological perturbations: The derivation of the second-order Einstein equation in a gauge-invariant manner without any gauge fixing[11]; Applicability in more generic situations[12]; Confirmation of the consistency between all components of the second-order Einstein equations and equations of motions[13]. We also note that the radiation case has recently been discussed by treating the Boltzmann equation up to second order[14] along the gauge-invariant manner of the above series of papers by the present author.

In this review article, we summarize the current status of this development of the second-order gauge-invariant cosmological perturbation theory through the simple system of a sclar field. Through this review, we point out the problems which should be clarified and directions of the further development of the theoretical sophistication of the general relativistic higher-order perturbation theory, especially in cosmological perturbations. We expect that this sophistication will be also useful to discuss the theoretical predictions of Non-Gaussianity in CMB and comparison with observations.

The organization of this paper is as follows. In Sec. II, we review the general framework of the second-order gauge invariant perturbation theory developed in Refs. [8, 9, 11, 15]. This review also includes additional explanation not given in those papers. In Sec. III, we also the derivations of the second-order perturbation of the Einstein equation and the energy-momentum tensor from general point of view. For simplicity, in this paper, we only consider a single scalar field as a matter content. The ingredients of Sec. II and III will be applicable to perturbation theory in any theory with general covariance, if the decomposition formula (2.23) for the linear-order metric perturbation is correct. In Sec. IV, we summarize the Einstein equations in the case of a background homogeneous isotropic universe, which are used in the derivation of the first- and second-order Einstein equations. In Sec. V, the first-order perturbation of the Einstein equations and the Klein-Gordon equations are summarized. The derivation of the second-order perturbations of the Einstein equations and the Klein-Gordon equations, and their consistency are reviewed in Sec. VI. The final section, Sec. VII, is devoted to a summary and discussions.

II. GENERAL FRAMEWORK OF THE GENERAL RELATIVISTIC GAUGE-INVARIANT PERTURBATION THEORY

In this section, we review the general framework of the gauge invariant perturbation theory developed in Refs. [8–11, 15–21]. To develop the general relativistic

gauge-invariant perturbation theory, we first explain the general arguments of the Taylor expansion on a manifold without introducing an explicit coordinate system in Sec.II A. Further, we also have to clarify the notion of "gauge" in general relativity to develop the gauge-invariant perturbation theory from general point of view, which is explained in Sec. II B. After clarifying the notion of "gauge" in general relativistic perturbations, in Sec. II C, we explain the formulation of the general relativistic gauge-invariant perturbation theory from general point of view. Although our understanding of "gauge" in general relativistic perturbations essentially is different from "degree of freedom of coordinates" as in many literature, "a coordinate transformation" is induced by our understanding of "gauge". This situation is explained in Sec. II D. To exclude "gauge degree of freedom" which is unphysical degree of freedom in perturbations, we construct "gauge-invariant variables" of perturbations as reviewed in Sec. II E. These "gauge-invariant variables" are regarded as physical quantities.

A. Taylor expansion of tensors on a manifold

First, we briefly review the issues on the general form of the Taylor expansion of tensors on a manifold $\mathcal{M}$. The gauge issue of general relativistic perturbation theories which we will discuss is related to the coordinate transformation. Therefore, we have to discuss the general form of the Taylor expansion without the explicit introduction of coordinate systems. Although we only consider the Taylor expansion of a scalar function $f : \mathcal{M} \mapsto \mathbb{R}$, here, the resulting formula is extended to that for any tensor field on a manifold as in Appendix A. We have to emphasize that the general formula of the Taylor expansion shown here is the starting point of our gauge-invariant formulation of the second-order general relativistic perturbation theory.

The Taylor expansion of a function f is an approximated form of $f(q)$ at $q \in \mathcal{M}$ in terms of the variables at $p \in \mathcal{M}$, where q is in the neighborhood of p. To derive the formula for the Taylor expansion of f, we have to compare the values of f at the different points on the manifold. To accomplish this, we introduce a one-parameter family of diffeomorphisms $\Phi_\lambda : \mathcal{M} \mapsto \mathcal{M}$, where $\Phi_\lambda(p) = q$ and $\Phi_{\lambda=0}(p) = p$. One example of a diffeomorphisms Φ_λ is an exponential map with a generator. However, we consider a more general class of diffeomorphisms.

The diffeomorphism Φ_λ induces the pull-back Φ^*_λ of the function f and this pull-back enable us to compare the values of the function f at different points. Further, the Taylor expansion of the function $f(q)$ is given by

$$\begin{aligned} f(q) &= f(\Phi_\lambda(p)) =: (\Phi^*_\lambda f)(p) \\ &= f(p) + \left.\frac{\partial}{\partial\lambda}(\Phi^*_\lambda f)\right|_p \lambda + \frac{1}{2}\left.\frac{\partial^2}{\partial\lambda^2}(\Phi^*_\lambda f)\right|_p \lambda^2 \\ &\quad +O(\lambda^3). \end{aligned} \tag{2.1}$$

Since this expression hold for an arbitrary smooth function f, the function f in Eq. (2.1) can be regarded as a dummy. Therefore, we may regard the Taylor expansion (2.1) to be the expansion of the pull-back Φ^*_λ of the diffeomorphism Φ_λ, rather than the expansion of the function f.

According to this point of view, Sonego and Bruni[18] showed that there exist vector fields ξ^a_1 and ξ^a_2 such that the expansion (2.1) is given by

$$\begin{aligned} f(q) &= (\Phi^*_\lambda f)(p) \\ &= f(p) + \left.(\pounds_{\xi_1} f)\right|_p \lambda + \frac{1}{2}\left.\left(\pounds_{\xi_2} + \pounds^2_{\xi_1}\right) f\right|_p \lambda^2 \\ &\quad +O(\lambda^3), \end{aligned} \tag{2.2}$$

without loss of generality (see Appendix A). Equation (2.2) is not only the representation of the Taylor expansion of the function f, but also the definitions of the generators ξ^a_1 and ξ^a_2. These generators of the one-parameter family of diffeomorphisms Φ_λ represent the direction along which the Taylor expansion is carried out. The generator ξ^a_1 is the first-order approximation of the flow of the diffeomorphism Φ_λ, and the generator ξ^a_2 is the second-order correction to this flow. We should regard the generators ξ^a_1 and ξ^a_2 to be independent. Further, as shown in Appendix A, the representation of the Taylor expansion of an arbitrary scalar function f is extended to that for an arbitrary tensor field Q just through the replacement $f \to Q$.

We must note that, in general, the representation (2.2) of the Taylor expansion is different from an usual exponential map which is generated by a vector field. In general,

$$\Phi_\sigma \circ \Phi_\lambda \neq \Phi_{\sigma+\lambda}, \quad \Phi^{-1}_\lambda \neq \Phi_{-\lambda}. \tag{2.3}$$

As noted in Ref. [10], if the second-order generator ξ_2 in Eq. (2.2) is proportional to the first-order generator ξ_1 in Eq. (2.2), the diffeomorphism Φ_λ is reduced to an exponential map. Therefore, one may reasonably doubt that Φ_λ forms a group except under very special conditions. However, we have to note that the properties (2.3) does not directly mean that Φ_λ does not form a group. There will be possibilities that Φ_λ form a group in a different sense from exponential maps, in which the properties (2.3) will be maintained.

Now, we give an intuitive explanation of the representation (2.2) of the Taylor expansion through the case where the scalar function f in Eq. (2.2) is a coordinate function. When two points $p, q \in \mathcal{M}$ in Eq. (2.2) are in the neighborhood of each other, we can apply a coordinate system $\mathcal{M} \mapsto \mathbb{R}^n$ ($n = \dim\mathcal{M}$), which denoted by $\{x^\mu\}$, to an open set which includes these two points. Then, we can measure the relative position of these two points p and q in $\mathcal{M}$ in terms of this coordinate system in $\mathbb{R}^n$ through the Taylor expansion (2.2). In this case, we may regard that the scalar function f in Eq. (2.2) is

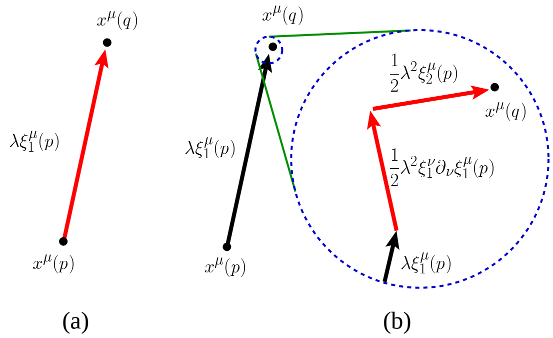

FIG. 1: (a) The second term $\lambda\xi_1(p)$ in Eq. (2.4) is the vector which point from the point $x^\mu(p)$ to the point $x^\mu(q)$ in the sense of the first-order correction. (b) If we look at the neighborhood of the point $x^\mu(q)$ in detail, the vector $\lambda\xi_1(p)$ may fail to point to $x^\mu(q)$ in the sense of the second order. Therefore, it is necessary to add the second-order correction $\frac{1}{2}\lambda^2(\xi_2^\mu + \xi_1^\nu(p)\partial_\nu\xi_1^\mu(p))$.

a coordinate function x^μ and Eq. (2.2) yields

$$\begin{aligned} x^\mu(q) &= (\Phi_\lambda^* x^\mu)(p) \\ &= x^\mu(p) + \lambda\xi_1(p) + \frac{1}{2}\lambda^2 \left(\xi_2 + \xi_1^\nu\partial_\nu\xi_1^\mu\right)\big|_p \\ &\quad + O(\lambda^3), \end{aligned} \tag{2.4}$$

The second term $\lambda\xi_1(p)$ in the right hand side of Eq. (2.4) is familiar. This is regarded as the vector which point from the point $x^\mu(p)$ to the point $x^\mu(q)$ in the sense of the first-order correction as shown in Fig.1(a). However, in the sense of the second order, this vector $\lambda\xi_1(p)$ may fail to point to $x^\mu(q)$. Therefore, it is necessary to add the second-order correction as shown in Fig.1(b). As a correction of the second order, we may add the term $\frac{1}{2}\lambda^2\xi_1^\nu(p)\partial_\nu\xi_1^\mu(p)$. This second-order correction corresponds to that comes from the exponential map which is generated by the vector field ξ_1^μ. However, this correction completely determined by the vector field ξ_1^μ. Even if we add this correction comes from the exponential map, there is no guarantee that the corrected vector $\lambda\xi_1(p)+\frac{1}{2}\lambda^2\xi_1^\nu(p)\partial_\nu\xi_1^\mu(p)$ does point to $x^\mu(q)$ in the sense of the second order Thus, we have to add the new correction $\frac{1}{2}\lambda^2\xi_2^\nu(p)$ of the second order, in general.

Of course, without this correction $\frac{1}{2}\lambda^2\xi_2^\nu(p)$, the vector which comes only from the exponential map generated by the vector field ξ_1 might point to the point $x^\mu(q)$. Actually, this is possible if we carefully choose the vector field ξ_1^μ taking into account of the deviations at the second order. However, this means that we have to take care of the second-order correction when we determine the first-order correction. This contradicts to the philosophy of the Taylor expansion as a perturbative expansion, in which we can determine everything order by order. Therefore, we should regard that the correction $\frac{1}{2}\lambda^2\xi_2^\nu(p)$ is necessary in general situations.

B. Gauge degree of freedom in general relativity

Since we want to explain the gauge-invariant perturbation theory in general relativity, first of all, we have to explain the notion of "gauge" in general relativity[15]. General relativity is a theory with general covariance, which intuitively states that there is no preferred coordinate system in nature. This general covariance also introduce the notion of "gauge" in the theory. In the theory with general covariance, these "gauge" give rise to the unphysical degree of freedom and we have to fix the "gauges" or to extract some invariant quantities to obtain physical result. Therefore, treatments of "gauges" are crucial in general relativity and this situation becomes more delicate in general relativistic perturbation theory as explained below.

In 1964, Sachs[16] pointed out that there are two kinds of "gauges" in general relativity. Sachs called these two "gauges" as the first- and the second-kind of gauges, respectively. Here, we review these concepts of "gauge".

1. *First kind gauge*

The first kind gauge is a coordinate system on a single manifold $\mathcal{M}$. Although this first kind gauge is not important in this paper, we explain this to emphasize the "gauge" discussing in this paper is different from this first kind gauge.

In the standard text book of manifolds (for example, see [23]), the following property of a manifold is written: on a manifold, we can always introduce a coordinate system as a diffeomorphism ψ_α from an open set $O_\alpha \subset \mathcal{M}$ to an open set $\psi_\alpha(O_\alpha) \subset \mathbb{R}^n$ ($n = \dim \mathcal{M}$). This diffeomorphism ψ_α, i.e., coordinate system of the open set O_α, is called *gauge choice* (of the first kind). If we consider another open set in $O_\beta \subset \mathcal{M}$, we have another gauge choice $\psi_\beta : O_\beta \mapsto \psi_\beta(O_\beta) \subset \mathbb{R}^n$ for O_β. If these two open sets O_α and O_β have the intersection $O_\alpha \cap O_\beta \neq \emptyset$, we can consider the diffeomorphism $\psi_\beta \circ \psi_\alpha^{-1}$. This diffeomorphism $\psi_\beta \circ \psi_\alpha^{-1}$ is just a coordinate transformation: $\psi_\alpha(O_\alpha \cap O_\beta) \subset \mathbb{R}^n \mapsto \psi_\beta(O_\alpha \cap O_\beta) \subset \mathbb{R}^n$, which is called *gauge transformation* (of the first kind) in general relativity.

According to the theory of a manifold, coordinate system are not on a manifold itself but we can always introduce a coordinate system through a map from an open set in the manifold $\mathcal{M}$ to an open set of $\mathbb{R}^n$. For this reason, general covariance in general relativity is automatically included in the premise that our spacetime is regarded as a single manifold. The first kind gauge does arise due to this general covariance. The gauge issue of the first kind is represented by the question, which coordinate system is convenient? The answer to this question depends on the problem which we are addressing, i.e., what we want to clarify. In some case, this gauge issue of the first kind is an important. However, in many case, it becomes harmless if we apply a covariant theory on the manifold.

2. Second kind gauge

The second kind gauge appears in perturbation theories in a theory with general covariance. This notion of the second kind "gauge" is the main issue of this paper. To explain this, we have to remind what we are doing in perturbation theories.

First, in any perturbation theories, we always treat two spacetime manifolds. One is the physical spacetime $\mathcal{M}$. This physical spacetime $\mathcal{M}$ is our nature itself and we want to describe the properties of this physical spacetime $\mathcal{M}$ through perturbations. The other is the background spacetime $\mathcal{M}_0$. This background spacetime have nothing to do with our nature and this is a fictitious manifold which is prepared by us. This background spacetime is just a reference to carry out perturbative analyses. We emphasize that these two spacetime manifolds $\mathcal{M}$ and $\mathcal{M}_0$ are distinct. Let us denote the physical spacetime by $(\mathcal{M}, \bar{g}_{ab})$ and the background spacetime by $(\mathcal{M}_0, g_{ab})$, where $\bar{g}_{ab}$ is the metric on the physical spacetime manifold, $\mathcal{M}$, and g_{ab} is the metric on the background spacetime manifold, $\mathcal{M}_0$. Further, we formally denote the spacetime metric and the other physical tensor fields on $\mathcal{M}$ by Q and its background value on $\mathcal{M}_0$ by Q_0.

Second, in any perturbation theories, we always write equations for the perturbation of the physical variable Q in the form

$$Q(\text{“}p\text{”}) = Q_0(p) + \delta Q(p). \tag{2.5}$$

Usually, this equation is simply regarded as a relation between the physical variable Q and its background value Q_0, or as the definition of the deviation δQ of the physical variable Q from its background value Q_0. However, Eq. (2.5) has deeper implications. Keeping in our mind that we always treat two different spacetimes, $\mathcal{M}$ and $\mathcal{M}_0$, in perturbation theory, Eq. (2.5) is a rather curious equation in the following sense: The variable on the left-hand side of Eq. (2.5) is a variable on $\mathcal{M}$, while the variables on the right-hand side of Eq. (2.5) are variables on $\mathcal{M}_0$. Hence, Eq. (2.5) gives a relation between variables on two different manifolds.

Further, through Eq. (2.5), we have implicitly identified points in these two different manifolds. More specifically, $Q(\text{“}p\text{”})$ on the left-hand side of Eq. (2.5) is a field on $\mathcal{M}$, and "p" $\in \mathcal{M}$. Similarly, we should regard the background value $Q_0(p)$ of $Q(\text{“}p\text{”})$ and its deviation $\delta Q(p)$ of $Q(\text{“}p\text{”})$ from $Q_0(p)$, which are on the right-hand side of Eq. (2.5), as fields on $\mathcal{M}_0$, and $p \in \mathcal{M}_0$. Because Eq. (2.5) is regarded as an equation for field variables, it implicitly states that the points "p" $\in \mathcal{M}$ and $p \in \mathcal{M}_0$ are same. This represents the implicit assumption of the existence of a map $\mathcal{M}_0 \to \mathcal{M} : p \in \mathcal{M}_0 \mapsto$ "p" $\in \mathcal{M}$, which is usually called a *gauge choice* (of the second kind) in perturbation theory[17].

It is important to note that the second kind gauge choice between points on $\mathcal{M}_0$ and $\mathcal{M}$, which is established by such a relation as Eq. (2.5), is not unique to the theory with general covariance. Rather, Eq. (2.5) involves the degree of freedom corresponding to the choice of the map $\mathcal{X} : \mathcal{M}_0 \mapsto \mathcal{M}$. This is called the *gauge degree of freedom* (of the second kind). Such a degree of freedom always exists in perturbations of a theory with general covariance. General covariance intuitively means that there is no preferred coordinate system in the theory as mentioned above. If general covariance is not imposed on the theory, there is a preferred coordinate system in the theory, and we naturally introduce this preferred coordinate system onto both $\mathcal{M}_0$ and $\mathcal{M}$. Then, we can choose the identification map $\mathcal{X}$ using this preferred coordinate system. However, there is no such coordinate system in general relativity due to the general covariance, and we have no guiding principle to choose the identification map $\mathcal{X}$. Indeed, we may identify "p" $\in \mathcal{M}$ with $q \in \mathcal{M}_0$ ($q \neq p$) instead of $p \in \mathcal{M}_0$. In the above understanding of the concept of "gauge" (of the second kind) in general relativistic perturbation theory, a gauge transformation is simply a change of the map $\mathcal{X}$.

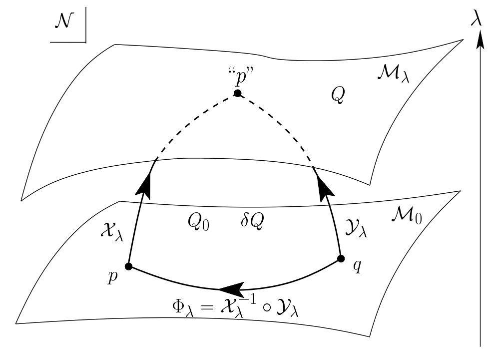

FIG. 2: The second kind gauge is a point-identification between the physical spacetime $\mathcal{M}_\lambda$ and the background spacetime $\mathcal{M}_0$ on the extended manifold $\mathcal{N}$. Through Eq. (2.5), we implicitly assume the existence of a point-identification map between $\mathcal{M}_\lambda$ and $\mathcal{M}_0$. However, this point-identification is not unique by virtue of the general covariance in the theory. We may chose the gauge of the second kind so that $p \in \mathcal{M}_0$ and "p"$\in \mathcal{M}_\lambda$ is same ($\mathcal{X}_\lambda$). We may also choose the gauge so that $q \in \mathcal{M}_0$ and "p"$\in \mathcal{M}_\lambda$ is same ($\mathcal{Y}_\lambda$). These are different gauge choices. The gauge transformation $\mathcal{X}_\lambda \to \mathcal{Y}_\lambda$ is given by the diffeomorphism $\Phi = \mathcal{X}_\lambda^{-1} \circ \mathcal{Y}_\lambda$.

These are the basic ideas of gauge degree of freedom (of the second kind) in the general relativistic perturbation theory which are pointed out by Sacks[16] and mathematically clarified by Stewart and Walker[17]. Based on these ideas, higher-order perturbation theory has been developed in Refs. [8–13, 15, 20–22].

C. Formulation of perturbation theory

To formulate the above understanding in more detail, we introduce an infinitesimal parameter λ for the perturbation. Further, we consider the 4 + 1-dimensional

manifold $\mathcal{N} = \mathcal{M} \times \mathbb{R}$, where $4 = \dim \mathcal{M}$ and $\lambda \in \mathbb{R}$. The background spacetime $\mathcal{M}_0 = \mathcal{N}|_{\lambda=0}$ and the physical spacetime $\mathcal{M} = \mathcal{M}_\lambda = \mathcal{N}|_{\mathbb{R}=\lambda}$ are also submanifolds embedded in the extended manifold $\mathcal{N}$. Each point on $\mathcal{N}$ is identified by a pair (p, λ), where $p \in \mathcal{M}_\lambda$, and each point in $\mathcal{M}_0 \subset \mathcal{N}$ is identified by $\lambda = 0$.

Through this construction, the manifold $\mathcal{N}$ is foliated by four-dimensional submanifolds $\mathcal{M}_\lambda$ of each λ, and these are diffeomorphic to $\mathcal{M}$ and $\mathcal{M}_0$. The manifold $\mathcal{N}$ has a natural differentiable structure consisting of the direct product of $\mathcal{M}$ and $\mathbb{R}$. Further, the perturbed spacetimes $\mathcal{M}_\lambda$ for each λ must have the same differential structure with this construction. In other words, we require that perturbations be continuous in the sense that $\mathcal{M}$ and $\mathcal{M}_0$ are connected by a continuous curve within the extended manifold $\mathcal{N}$. Hence, the changes of the differential structure resulting from the perturbation, for example the formation of singularities and singular perturbations in the sense of fluid mechanics, are excluded from consideration.

Let us consider the set of field equations

$$\mathcal{E}[Q_\lambda] = 0 \tag{2.6}$$

on the physical spacetime $\mathcal{M}_\lambda$ for the physical variables Q_λ on $\mathcal{M}_\lambda$. The field equation (2.6) formally represents the Einstein equation for the metric on $\mathcal{M}_\lambda$ and the equations for matter fields on $\mathcal{M}_\lambda$. If a tensor field Q_λ is given on each $\mathcal{M}_\lambda$, Q_λ is automatically extended to a tensor field on $\mathcal{N}$ by $Q(p, \lambda) := Q_\lambda(p)$, where $p \in \mathcal{M}_\lambda$. In this extension, the field equation (2.6) is regarded as an equation on the extended manifold $\mathcal{N}$. Thus, we have extended an arbitrary tensor field and the field equations (2.6) on each $\mathcal{M}_\lambda$ to those on the extended manifold $\mathcal{N}$.

Tensor fields on $\mathcal{N}$ obtained through the above construction are necessarily "tangent" to each $\mathcal{M}_\lambda$. To consider the basis of the tangent space of $\mathcal{N}$, we introduce the normal form and its dual, which are normal to each $\mathcal{M}_\lambda$ in $\mathcal{N}$. These are denoted by $(d\lambda)_a$ and $(\partial/\partial\lambda)^a$, respectively, and they satisfy $(d\lambda)_a(\partial/\partial\lambda)^a = 1$. The form $(d\lambda)_a$ and its dual, $(\partial/\partial\lambda)^a$, are normal to any tensor field extended from the tangent space on each $\mathcal{M}_\lambda$ through the above construction. The set consisting of $(d\lambda)_a$, $(\partial/\partial\lambda)^a$ and the basis of the tangent space on each $\mathcal{M}_\lambda$ is regarded as the basis of the tangent space of $\mathcal{N}$.

Now, we define the perturbation of an arbitrary tensor field Q. We compare Q on $\mathcal{M}_\lambda$ with Q_0 on $\mathcal{M}_0$, and it is necessary to identify the points of $\mathcal{M}_\lambda$ with those of $\mathcal{M}_0$ as mentioned above. This point identification map is the gauge choice of the second kind as mentioned above. The gauge choice is made by assigning a diffeomorphism $\mathcal{X}_\lambda : \mathcal{N} \to \mathcal{N}$ such that $\mathcal{X}_\lambda : \mathcal{M}_0 \to \mathcal{M}_\lambda$. Following the paper of Bruni et al.[10], we introduce a gauge choice $\mathcal{X}_\lambda$ as an one-parameter groups of diffeomorphisms, i.e., an exponential map, for simplicity. We denote the generator of this exponential map by ${}_{\mathcal{X}}\eta^a$. This generator ${}_{\mathcal{X}}\eta^a$ is decomposed by the basis on $\mathcal{N}$ which are constructed above. Although the generator ${}_{\mathcal{X}}\eta^a$ should satisfy some appropriate properties[8], the arbitrariness of the gauge choice $\mathcal{X}_\lambda$ is represented by the tangential component of the generator ${}_{\mathcal{X}}\eta^a$ to $\mathcal{M}_\lambda$.

The pull-back $\mathcal{X}^*_\lambda Q$, which is induced by the exponential map $\mathcal{X}_\lambda$, maps a tensor field Q on the physical manifold $\mathcal{M}_\lambda$ to a tensor field $\mathcal{X}^*_\lambda Q$ on the background spacetime. In terms of this generator ${}_{\mathcal{X}}\eta^a$, the pull-back $\mathcal{X}^*_\lambda Q$ is represented by the Taylor expansion

$$\begin{aligned} Q(r) &= Q(\mathcal{X}_\lambda(p)) = \mathcal{X}^*_\lambda Q(p) \\ &= Q(p) + \lambda \left.\pounds_{{}_{\mathcal{X}}\eta} Q\right|_p + \frac{1}{2}\lambda^2 \left.\pounds^2_{{}_{\mathcal{X}}\eta} Q\right|_p \\ &\quad +O(\lambda^3), \end{aligned} \tag{2.7}$$

where $r = \mathcal{X}_\lambda(p) \in \mathcal{M}_\lambda$. Because $p \in \mathcal{M}_0$, we may regard the equation

$$\begin{aligned} \mathcal{X}^*_\lambda Q(p) &= Q_0(p) + \lambda \left.\pounds_{{}_{\mathcal{X}}\eta} Q\right|_{\mathcal{M}_0}(p) + \frac{1}{2}\lambda^2 \left.\pounds^2_{{}_{\mathcal{X}}\eta} Q\right|_{\mathcal{M}_0}(p) \\ &\quad +O(\lambda^3) \end{aligned} \tag{2.8}$$

as an equation on the background spacetime $\mathcal{M}_0$, where $Q_0 = Q|_{\mathcal{M}_0}$ is the background value of the physical variable of Q. Once the definition of the pull-back of the gauge choice $\mathcal{X}_\lambda$ is given, the first- and the second-order perturbations ${}^{(1)}_{\mathcal{X}}Q$ and ${}^{(2)}_{\mathcal{X}}Q$ of a tensor field Q under the gauge choice $\mathcal{X}_\lambda$ are simply given by the expansion

$$\left.\mathcal{X}^*_\lambda Q_\lambda\right|_{\mathcal{M}_0} = Q_0 + \lambda {}^{(1)}_{\mathcal{X}}Q + \frac{1}{2}\lambda^2 {}^{(2)}_{\mathcal{X}}Q + O(\lambda^3) \tag{2.9}$$

with respect to the infinitesimal parameter λ. Comparing Eqs. (2.8) and (2.9), we define the first- and the second-order perturbations of a physical variable Q_λ under the gauge choice $\mathcal{X}_\lambda$ by

$${}^{(1)}_{\mathcal{X}}Q := \left.\pounds_{{}_{\mathcal{X}}\eta} Q\right|_{\mathcal{M}_0}, \quad {}^{(2)}_{\mathcal{X}}Q := \left.\pounds^2_{{}_{\mathcal{X}}\eta} Q\right|_{\mathcal{M}_0}. \tag{2.10}$$

We note that all variables in Eq. (2.9) are defined on $\mathcal{M}_0$.

Now, we consider two *different gauge choices* based on the above understanding of the second kind gauge choice. Suppose that $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ are two exponential maps with the generators ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ on $\mathcal{N}$, respectively. In other words, $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ are two gauge choices (see Fig. 2). Then, the integral curves of each ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ in $\mathcal{N}$ are the orbits of the actions of the gauge choices $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$, respectively. Since we choose the generators ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ so that these are transverse to each $\mathcal{M}_\lambda$ everywhere on $\mathcal{N}$, the integral curves of these vector fields intersect with each $\mathcal{M}_\lambda$. Therefore, points lying on the same integral curve of either of the two are to be regarded as *the same point* within the respective gauges. When these curves are not identical, i.e., the tangential components to each $\mathcal{M}_\lambda$ of ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ are different, these point identification maps $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ are regarded as *two different gauge choices*.

We next introduce the concept of *gauge invariance*. In particular, in this paper, we consider the concept of *order by order gauge invariance*[12]. Suppose that $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$

are two different gauge choices which are generated by the vector fields ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$, respectively. These gauge choices also pull back a generic tensor field Q on $\mathcal{N}$ to two other tensor fields, $\mathcal{X}^*_\lambda Q$ and $\mathcal{Y}^*_\lambda Q$, for any given value of λ. In particular, on $\mathcal{M}_0$, we now have three tensor fields associated with a tensor field Q; one is the background value Q_0 of Q, and the other two are the pulled-back variables of Q from $\mathcal{M}_\lambda$ to $\mathcal{M}_0$ by the two different gauge choices,

$$\begin{aligned} {}_{\mathcal{X}}Q_\lambda &:= \mathcal{X}^*_\lambda Q|_{\mathcal{M}_0} \\ &= Q_0 + \lambda {}^{(1)}_{\mathcal{X}}Q + \frac{1}{2}\lambda^2 {}^{(2)}_{\mathcal{X}}Q + O(\lambda^3) \qquad (2.11) \\ {}_{\mathcal{Y}}Q_\lambda &:= \mathcal{Y}^*_\lambda Q|_{\mathcal{M}_0} \\ &= Q_0 + \lambda {}^{(1)}_{\mathcal{Y}}Q + \frac{1}{2}\lambda^2 {}^{(2)}_{\mathcal{Y}}Q + O(\lambda^3) \qquad (2.12) \end{aligned}$$

Here, we have used Eq. (2.9). Because $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ are gauge choices which map from $\mathcal{M}_0$ to $\mathcal{M}_\lambda$, ${}_{\mathcal{X}}Q_\lambda$ and ${}_{\mathcal{Y}}Q_\lambda$ are the different representations on $\mathcal{M}_0$ in the two different gauges of the same perturbed tensor field Q on $\mathcal{M}_\lambda$. The quantities ${}^{(k)}_{\mathcal{X}}Q$ and ${}^{(k)}_{\mathcal{Y}}Q$ in Eqs. (2.11) and (2.12) are the perturbations of $O(k)$ in the gauges $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$, respectively. We say that the kth-order perturbation ${}^{(k)}_{\mathcal{X}}Q$ of Q is *order by order gauge invariant* iff for any two gauges $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ the following holds:

$$ {}^{(k)}_{\mathcal{X}}Q = {}^{(k)}_{\mathcal{Y}}Q. \qquad (2.13)$$

Now, we consider the *gauge transformation rules* between different gauge choices. In general, the representation ${}^{\mathcal{X}}Q_\lambda$ on $\mathcal{M}_0$ of the perturbed variable Q on $\mathcal{M}_\lambda$ depends on the gauge choice $\mathcal{X}_\lambda$. If we employ a different gauge choice, the representation of Q_λ on $\mathcal{M}_0$ may change. Suppose that $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$ are different gauge choices, which are the point identification maps from $\mathcal{M}_0$ to $\mathcal{M}_\lambda$, and the generators of these gauge choices are given by ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$, respectively. Then, the change of the gauge choice from $\mathcal{X}_\lambda$ to $\mathcal{Y}_\lambda$ is represented by the diffeomorphism

$$\Phi_\lambda := (\mathcal{X}_\lambda)^{-1} \circ \mathcal{Y}_\lambda. \qquad (2.14)$$

This diffeomorphism Φ_λ is the map $\Phi_\lambda : \mathcal{M}_0 \to \mathcal{M}_0$ for each value of $\lambda \in \mathbb{R}$. The diffeomorphism Φ_λ does change the point identification, as expected from the understanding of the gauge choice discussed above. Therefore, the diffeomorphism Φ_λ is regarded as the gauge transformation $\Phi_\lambda : \mathcal{X}_\lambda \to \mathcal{Y}_\lambda$.

The gauge transformation Φ_λ induces a pull-back from the representation ${}_{\mathcal{X}}Q_\lambda$ of the perturbed tensor field Q in the gauge choice $\mathcal{X}_\lambda$ to the representation ${}_{\mathcal{Y}}Q_\lambda$ in the gauge choice $\mathcal{Y}_\lambda$. Actually, the tensor fields ${}_{\mathcal{X}}Q_\lambda$ and ${}_{\mathcal{Y}}Q_\lambda$, which are defined on $\mathcal{M}_0$, are connected by the linear map Φ^*_λ as

$$\begin{aligned} {}_{\mathcal{Y}}Q_\lambda &= \mathcal{Y}^*_\lambda Q|_{\mathcal{M}_0} = \left.\left(\mathcal{Y}^*_\lambda \left(\mathcal{X}_\lambda \mathcal{X}^{-1}_\lambda\right)^* Q\right)\right|_{\mathcal{M}_0} \\ &= \left(\mathcal{X}^{-1}_\lambda \mathcal{Y}_\lambda\right)^* \left.\left(\mathcal{X}^*_\lambda Q\right)\right|_{\mathcal{M}_0} = \Phi^*_\lambda {}_{\mathcal{X}}Q_\lambda. \qquad (2.15) \end{aligned}$$

According to generic arguments concerning the Taylor expansion of the pull-back of a tensor field on the same manifold, given in §II A, it should be possible to express the gauge transformation $\Phi^*_\lambda {}_{\mathcal{X}}Q_\lambda$ in the form

$$\begin{aligned} \Phi^*_\lambda {}_{\mathcal{X}}Q = {}_{\mathcal{X}}Q + \lambda \pounds_{\xi_1} {}_{\mathcal{X}}Q + \frac{\lambda^2}{2}\left\{\pounds_{\xi_2} + \pounds^2_{\xi_1}\right\} {}_{\mathcal{X}}Q \\ + O(\lambda^3), \quad (2.16) \end{aligned}$$

where the vector fields ξ^a_1 and ξ^a_2 are the generators of the gauge transformation Φ_λ (see Eq. (2.2)).

Comparing the representation (2.16) of the Taylor expansion in terms of the generators ξ^a_1 and ξ^a_2 of the pull-back $\Phi^*_\lambda {}_{\mathcal{X}}Q$ and that in terms of the generators ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ of the pull-back $\mathcal{Y}^*_\lambda \circ \left(\mathcal{X}^{-1}_\lambda\right)^* {}_{\mathcal{X}}Q$ $(= \Phi^*_\lambda {}_{\mathcal{X}}Q)$, we readily obtain explicit expressions for the generators ξ^a_1 and ξ^a_2 of the gauge transformation $\Phi = \mathcal{X}^{-1}_\lambda \circ \mathcal{Y}_\lambda$ in terms of the generators ${}_{\mathcal{X}}\eta^a$ and ${}_{\mathcal{Y}}\eta^a$ of each gauge choices as follows:

$$\xi^a_1 = {}_{\mathcal{Y}}\eta^a - {}_{\mathcal{X}}\eta^a, \quad \xi^a_2 = \left[{}_{\mathcal{Y}}\eta, {}_{\mathcal{X}}\eta\right]^a. \qquad (2.17)$$

Further, because the gauge transformation Φ_λ is a map within the background spacetime $\mathcal{M}_0$, the generator should consist of vector fields on $\mathcal{M}_0$. This can be satisfied by imposing some appropriate conditions on the generators ${}_{\mathcal{Y}}\eta^a$ and ${}_{\mathcal{X}}\eta^a$.

We can now derive the relation between the perturbations in the two different gauges. Up to second order, these relations are derived by substituting (2.11) and (2.12) into (2.16):

$$\begin{aligned} {}^{(1)}_{\mathcal{Y}}Q - {}^{(1)}_{\mathcal{X}}Q &= \pounds_{\xi_1} Q_0, \qquad (2.18) \\ {}^{(2)}_{\mathcal{Y}}Q - {}^{(2)}_{\mathcal{X}}Q &= 2\pounds_{\xi_1} {}^{(1)}_{\mathcal{X}}Q + \left\{\pounds_{\xi_2} + \pounds^2_{\xi_1}\right\} Q_0. \qquad (2.19) \end{aligned}$$

Here, we should comment on the gauge choice in the above explanation. We have introduced an exponential map $\mathcal{X}_\lambda$ (or $\mathcal{Y}_\lambda$) as the gauge choice, for simplicity. However, this simplified introduction of $\mathcal{X}_\lambda$ as an exponential map is not essential to the gauge transformation rules (2.18) and (2.19). Actually, we can generalize the diffeomorphism $\mathcal{X}_\lambda$ from an exponential map. For example, the diffeomorphism whose pull-back is represented by the Taylor expansion (2.2) is a candidate of the generalization. If we generalize the diffeomorphism $\mathcal{X}_\lambda$, the representation (2.8) of the pulled-back variable $\mathcal{X}^*_\lambda Q(p)$, the representations of the perturbations (2.10), and the relations (2.17) between generators of Φ_λ, $\mathcal{X}_\lambda$, and $\mathcal{Y}_\lambda$ will be changed. However, the gauge transformation rules (2.18) and (2.19) are direct consequences of the generic Taylor expansion (2.16) of Φ_λ. Generality of the representation of the Taylor expansion (2.16) of Φ_λ implies that the gauge transformation rules (2.18) and (2.19) will not be changed, even if we generalize the each gauge choice $\mathcal{X}_\lambda$. Further, the relations (2.17) between generators also imply that, even if we employ simple exponential maps as gauge choices, both of the generators ξ^a_1 and ξ^a_2 are naturally induced by the generators of the original gauge

choices. Hence, we conclude that the gauge transformation rules (2.18) and (2.19) are quite general and irreducible. In this paper, we review the development of a second-order gauge-invariant cosmological perturbation theory based on the above understanding of the gauge degree of freedom only through the gauge transformation rules (2.18) and (2.19). Hence, the developments of the cosmological perturbation theory presented below will not be changed even if we generalize the gauge choice $\mathcal{X}_\lambda$ from a simple exponential map.

We also have to emphasize the physical implication of the gauge transformation rules (2.18) and (2.19). According to the above construction of the perturbation theory, gauge degree of freedom, which induces the transformation rules (2.18) and (2.19), is unphysical degree of freedom. As emphasized above, the physical spacetime $\mathcal{M}_\lambda$ is our nature itself, while there is no background spacetime $\mathcal{M}_0$ in our nature. The background spacetime $\mathcal{M}_0$ is a fictitious spacetime and it have nothing to do with our nature. Since the gauge choice $\mathcal{X}_\lambda$ just gives a relation between $\mathcal{M}_\lambda$ and $\mathcal{M}_0$, the gauge choice $\mathcal{X}_\lambda$ also have nothing to do with our nature. On the other hand, any observations and experiments are carried out only on the physical spacetime $\mathcal{M}_\lambda$ through the physical processes on the physical spacetime $\mathcal{M}_\lambda$. Therefore, any direct observables in any observations and experiments should be independent of the gauge choice $\mathcal{X}_\lambda$, i.e., should be gauge invariant. Keeping this fact in our mind, the gauge transformation rules (2.18) and (2.19) imply that the perturbations ${}^{(1)}_{\mathcal{X}}Q$ and ${}^{(2)}_{\mathcal{X}}Q$ include unphysical degree of freedom, i.e., gauge degree of freedom, if these perturbations are transformed as (2.18) or (2.19) under the gauge transformation $\mathcal{X}_\lambda \to \mathcal{Y}_\lambda$. If the perturbations ${}^{(1)}_{\mathcal{X}}Q$ and ${}^{(2)}_{\mathcal{X}}Q$ are independent of the gauge choice, these variables are order by order gauge invariant. Therefore, order by order gauge-invariant variables does not include unphysical degree of freedom and should be related to the physics on the physical spacetime $\mathcal{M}_\lambda$.

D. Coordinate transformations induced by the second kind gauge transformation

In many literature, gauge degree of freedom is regarded as the degree of freedom of the coordinate transformation. In the linear-order perturbation theory, these two degree of freedom are equivalent with each other. However, in the higher order perturbations, we should regard that these two degree of freedom are different. Although the essential understanding of the gauge degree of freedom (of the second kind) is as that explained above, the gauge transformation (of the second kind) also induces the infinitesimal coordinate transformation on the physical spacetime $\mathcal{M}_\lambda$ as a result. In many case, the understanding of "gauges" in perturbations based on coordinate transformations leads mistakes. Therefore, we did not use any ingredient of this subsection in our series of papers[8, 9, 11–13] concerning about higher-order general relativistic gauge-invariant perturbation theory. However, we comment on the relations between the coordinate transformation, briefly. Details can be seen in Refs. [8, 19, 20].

To see that the gauge transformation of the second kind induces the coordinate transformation, we introduce the coordinate system $\{O_\alpha, \psi_\alpha\}$ on the "background spacetime" $\mathcal{M}_0$, where O_α are open sets on the background spacetime and ψ_α are diffeomorphisms from O_α to $\mathbb{R}^4$ ($4 = \dim \mathcal{M}_0$). The coordinate system $\{O_\alpha, \psi_\alpha\}$ is the set of the collection of the pair of open sets O_α and diffeomorphism $O_\alpha \mapsto \mathbb{R}^4$. If we employ a gauge choice $\mathcal{X}_\lambda$, we have the correspondence of $\mathcal{M}_\lambda$ and $\mathcal{M}_0$. Together with the coordinate system ψ_α on $\mathcal{M}_0$, this correspondence between $\mathcal{M}_\lambda$ and $\mathcal{M}_0$ induces the coordinate system on $\mathcal{M}_\lambda$. Actually, $X_\lambda(O_\alpha)$ for each α is an open set of $\mathcal{M}_\lambda$. Then, $\psi_\alpha \circ \mathcal{X}_\lambda^{-1}$ becomes a diffeomorphism from an open set $X_\lambda(O_\alpha) \subset \mathcal{M}_\lambda$ to $\mathbb{R}^4$. This diffeomorphism $\psi_\alpha \circ \mathcal{X}_\lambda^{-1}$ induces a coordinate system of an open set on $\mathcal{M}_\lambda$.

When we have two different gauge choices $\mathcal{X}_\lambda$ and $\mathcal{Y}_\lambda$, $\psi_\alpha \circ \mathcal{X}_\lambda^{-1}$ and $\psi_\alpha \circ \mathcal{Y}_\lambda^{-1}$ become different coordinate systems on $\mathcal{M}_\lambda$. We can also consider the coordinate transformation from the coordinate system $\psi_\alpha \circ \mathcal{X}_\lambda^{-1}$ to another coordinate system $\psi_\alpha \circ \mathcal{Y}_\lambda^{-1}$. Since the gauge transformation $\mathcal{X}_\lambda \to \mathcal{Y}_\lambda$ is induced by the diffeomorphism Φ_λ defined by Eq. (2.14), the induced coordinate transformation is given by

$$y^\mu(q) := x^\mu(p) = \left(\left(\Phi^{-1} \right)^* x^\mu \right)(q) \tag{2.20}$$

in the *passive* point of view[8, 19, 20]. If we represent this coordinate transformation in terms of the Taylor expansion in Sec. II A, up to third order, we have the coordinate transformation

$$\begin{aligned} y^\mu(q) &= x^\mu(q) - \lambda \xi_1^\mu(q) + \frac{\lambda^2}{2} \left\{ -\xi_2^\mu(q) + \xi_1^\nu(q) \partial_\nu \xi_1^\mu(q) \right\} \\ &\quad + O(\lambda^3). \end{aligned} \tag{2.21}$$

E. Gauge-invariant variables

Here, inspecting the gauge transformation rules (2.18) and (2.19), we define the gauge invariant variables for a metric perturbation and for arbitrary matter fields (tensor fields). Employing the idea of order by order gauge invariance for perturbations[12], we proposed a procedure to construct gauge invariant variables of higher-order perturbations[8]. This proposal is as follows. First, we decompose a linear-order metric perturbation into its gauge invariant and variant parts. The procedure for decomposing linear-order metric perturbations is extended to second-order metric perturbations, and we can decompose the second-order metric perturbation into gauge invariant and variant parts. Then, we can define the gauge invariant variables for the first- and second-order perturbations of an arbitrary field other than the metric by using the gauge variant parts of the first- and second-order

metric perturbations. Although the procedure for finding gauge invariant variables for linear-order metric perturbations is highly non-trivial, once we know this procedure, we can easily define the gauge invariant variables of a higher-order perturbation through a simple extension of the procedure for the linear-order perturbations.

Now, we review the above strategy to construct gauge-invariant variables. To consider a metric perturbation, we expand the metric on the physical spacetime $\mathcal{M}_\lambda$, which is pulled back to the background spacetime $\mathcal{M}_0$ using a gauge choice in the form given in (2.9):

$$\mathcal{X}^*_\lambda \bar{g}_{ab} \;=\; g_{ab} + \lambda\, {}_{\mathcal{X}}h_{ab} + \frac{\lambda^2}{2}\, {}_{\mathcal{X}}l_{ab} + O^3(\lambda), \quad (2.22)$$

where g_{ab} is the metric on $\mathcal{M}_0$. Of course, the expansion (2.22) of the metric depends entirely on the gauge choice $\mathcal{X}_\lambda$. Nevertheless, henceforth, we do not explicitly express the index of the gauge choice $\mathcal{X}_\lambda$ in an expression if there is no possibility of confusion.

Our starting point to construct gauge invariant variables is the assumption that *we already know the procedure for finding gauge invariant variables for the linear metric perturbations.* Then, a linear metric perturbation h_{ab} is decomposed as

$$h_{ab} =: \mathcal{H}_{ab} + \pounds_X g_{ab}, \quad (2.23)$$

where $\mathcal{H}_{ab}$ and X^a are the gauge invariant and variant parts of the linear-order metric perturbations, i.e., under the gauge transformation (2.18), these are transformed as

$${}_{\mathcal{Y}}\mathcal{H}_{ab} - {}_{\mathcal{X}}\mathcal{H}_{ab} = 0, \qquad {}_{\mathcal{Y}}X^a - {}_{\mathcal{X}}X^a = \xi_1^a. \quad (2.24)$$

The first-order metric perturbation (2.23) together with the gauge transformation rules (2.24) does satisfy the gauge transformation rule (2.18) for the first-order metric perturbation, i.e.,

$${}^{(1)}_{\mathcal{Y}}h_{ab} - {}^{(1)}_{\mathcal{X}}h_{ab} \;=\; \pounds_{\xi_1} g_{ab}. \quad (2.25)$$

As emphasized in our series of papers [8, 9, 11–13], the above assumption is quite non-trivial and it is not simple to carry out the systematic decomposition (2.23) on an arbitrary background spacetime, since this procedure depends completely on the background spacetime $(\mathcal{M}_0, g_{ab})$. However, as we will show below, this procedure exists at least in the case of cosmological perturbations of a homogeneous and isotropic universe in Sec. V A.

Once we accept this assumption for linear-order metric perturbations, we can always find gauge invariant variables for higher-order perturbations[8]. According to the gauge transformation rule (2.19), the second-order metric perturbation l_{ab} is transformed as

$${}^{(2)}_{\mathcal{Y}}l_{ab} - {}^{(2)}_{\mathcal{X}}l_{ab} = 2\pounds_{\xi_1}\, {}_{\mathcal{X}}h_{ab} + \left\{\pounds_{\xi_2} + \pounds^2_{\xi_1}\right\} g_{ab} \quad (2.26)$$

under the gauge transformation $\Phi_\lambda = (\mathcal{X}_\lambda)^{-1} \circ \mathcal{Y}_\lambda : \mathcal{X}_\lambda \to \mathcal{Y}_\lambda$. Although this gauge transformation rule is slightly complicated, inspecting this gauge transformation rule, we first introduce the variable $\hat{L}_{ab}$ defined by

$$\hat{L}_{ab} := l_{ab} - 2\pounds_X h_{ab} + \pounds^2_X g_{ab}. \quad (2.27)$$

Under the gauge transformation $\Phi_\lambda = (\mathcal{X}_\lambda)^{-1} \circ \mathcal{Y}_\lambda : \mathcal{X}_\lambda \to \mathcal{Y}_\lambda$, the variable $\hat{L}_{ab}$ is transformed as

$$\begin{aligned} {}_{\mathcal{Y}}\hat{L}_{ab} - {}_{\mathcal{X}}\hat{L}_{ab} \;&=\; \pounds_\sigma g_{ab}, & (2.28)\\ \sigma^a \;&:=\; \xi_2^a + [\xi_1, X]^a. & (2.29) \end{aligned}$$

The gauge transformation rule (2.28) is identical to that for a linear metric perturbation. Therefore, we may apply the above procedure to decompose h_{ab} into $\mathcal{H}_{ab}$ and X_a when we decompose of the components of the variable $\hat{L}_{ab}$. Then, $\hat{L}_{ab}$ can be decomposed as

$$\hat{L}_{ab} = \mathcal{L}_{ab} + \pounds_Y g_{ab}, \quad (2.30)$$

where $\mathcal{L}_{ab}$ is the gauge invariant part of the variable $\hat{L}_{ab}$, or equivalently, of the second-order metric perturbation l_{ab}, and Y^a is the gauge variant part of $\hat{L}_{ab}$, i.e., the gauge variant part of l_{ab}. Under the gauge transformation $\Phi_\lambda = (\mathcal{X}_\lambda)^{-1} \circ \mathcal{Y}_\lambda$, the variables $\mathcal{L}_{ab}$ and Y^a are transformed as

$${}_{\mathcal{Y}}\mathcal{L}_{ab} - {}_{\mathcal{X}}\mathcal{L}_{ab} = 0, \quad {}_{\mathcal{Y}}Y_a - {}_{\mathcal{Y}}Y_a = \sigma_a, \quad (2.31)$$

respectively. Thus, once we accept the assumption (2.23), the second-order metric perturbations are decomposed as

$$l_{ab} \;=:\; \mathcal{L}_{ab} + 2\pounds_X h_{ab} + \left(\pounds_Y - \pounds^2_X\right) g_{ab}, \quad (2.32)$$

where $\mathcal{L}_{ab}$ and Y^a are the gauge invariant and variant parts of the second order metric perturbations, i.e.,

$${}_{\mathcal{Y}}\mathcal{L}_{ab} - {}_{\mathcal{X}}\mathcal{L}_{ab} = 0, \quad {}_{\mathcal{Y}}Y^a - {}_{\mathcal{X}}Y^a = \xi_2^a + [\xi_1, X]^a. \quad (2.33)$$

Furthermore, as shown in Ref. [8], using the first- and second-order gauge variant parts, X^a and Y^a, of the metric perturbations, the gauge invariant variables for an arbitrary field Q other than the metric are given by

$$\begin{aligned} {}^{(1)}\mathcal{Q} \;&:=\; {}^{(1)}Q - \pounds_X Q_0, & (2.34)\\ {}^{(2)}\mathcal{Q} \;&:=\; {}^{(2)}Q - 2\pounds_X {}^{(1)}Q - \left\{\pounds_Y - \pounds^2_X\right\} Q_0. & (2.35) \end{aligned}$$

It is straightforward to confirm that the variables ${}^{(p)}\mathcal{Q}$ defined by (2.34) and (2.35) are gauge invariant under the gauge transformation rules (2.18) and (2.19), respectively.

Equations (2.34) and (2.35) have very important implications. To see this, we represent these equations as

$$\begin{aligned} {}^{(1)}Q \;&=\; {}^{(1)}\mathcal{Q} + \pounds_X Q_0, & (2.36)\\ {}^{(2)}Q \;&=\; {}^{(2)}\mathcal{Q} + 2\pounds_X {}^{(1)}Q + \left\{\pounds_Y - \pounds^2_X\right\} Q_0. & (2.37) \end{aligned}$$

These equations imply that any perturbation of first- and second-order can always be decomposed into gauge-invariant and gauge-variant parts as Eqs. (2.36) and (2.37), respectively. These decomposition formulae (2.36) and (2.37) are important ingredients in the general framework of the second-order general relativistic gauge-invariant perturbation theory.

III. PERTURBATIONS OF THE FIELD EQUATIONS

In terms of the gauge invariant variables defined last section, we derive the field equations, i.e., Einstein equations and the equation for a matter field. To derive the perturbation of the Einstein equations and the equation for a matter field (Klein-Gordon equation), first of all, we have to derive the perturbative expressions of the Einstein tensor[9]. This is reviewed in Sec. III A. We also derive the first- and the second-order perturbations of the energy momentum tensor for a scalar field and the Klein-Gordon equation[12] in Sec. III B. Finally, we consider the first- and the second-order the Einstein equations in Sec. III C.

A. Perturbations of the Einstein curvature

The relation between the curvatures associated with the metrics on the physical spacetime $\mathcal{M}_\lambda$ and the background spacetime $\mathcal{M}_0$ is given by the relation between the pulled-back operator $\mathcal{X}^*_\lambda\bar{\nabla}_a\left(\mathcal{X}^{-1}_\lambda\right)^*$ of the covariant derivative $\bar{\nabla}_a$ associated with the metric $\bar{g}_{ab}$ on $\mathcal{M}_\lambda$ and the covariant derivative ∇_a associated with the metric g_{ab} on $\mathcal{M}_0$. The pulled-back covariant derivative $\mathcal{X}^*_\lambda\bar{\nabla}_a\left(\mathcal{X}^{-1}_\lambda\right)^*$ depends on the gauge choice $\mathcal{X}_\lambda$. The property of the derivative operator $\mathcal{X}^*_\lambda\bar{\nabla}_a\left(\mathcal{X}^{-1}_\lambda\right)^*$ as the covariant derivative on $\mathcal{M}_\lambda$ is given by

$$\mathcal{X}^*_\lambda\bar{\nabla}_a\left(\left(\mathcal{X}^{-1}_\lambda\right)^*\mathcal{X}^*_\lambda\bar{g}_{ab}\right)=0, \tag{3.1}$$

where $\mathcal{X}^*_\lambda\bar{g}_{ab}$ is the pull-back of the metric on $\mathcal{M}_\lambda$, which is expanded as Eq. (2.22). In spite of the gauge dependence of the operator $\mathcal{X}^*_\lambda\bar{\nabla}_a\left(\mathcal{X}^{-1}_\lambda\right)^*$, we simply denote this operator by $\bar{\nabla}_a$, because our calculations are carried out only on $\mathcal{M}_0$ in the same gauge choice $\mathcal{X}_\lambda$. Further, we denote the pulled-back metric $\mathcal{X}^*_\lambda\bar{g}_{ab}$ on $\mathcal{M}_\lambda$ by $\bar{g}_{ab}$, as mentioned above.

Since the derivative operator $\bar{\nabla}_a$ $(=\mathcal{X}^*\bar{\nabla}_a\left(\mathcal{X}^{-1}\right)^*)$ may be regarded as a derivative operator on $\mathcal{M}_0$ that satisfies the property (3.1), there exists a tensor field $C^c{}_{ab}$ on $\mathcal{M}_0$ such that

$$\bar{\nabla}_a\omega_b=\nabla_a\omega_b-C^c{}_{ab}\omega_c, \tag{3.2}$$

where ω_a is an arbitrary one-form on $\mathcal{M}_0$. From the property (3.1) of the covariant derivative operator $\bar{\nabla}_a$ on $\mathcal{M}_\lambda$, the tensor field $C^c{}_{ab}$ on $\mathcal{M}_0$ is given by

$$C^c{}_{ab}=\frac{1}{2}\bar{g}^{cd}\left(\nabla_a\bar{g}_{db}+\nabla_b\bar{g}_{da}-\nabla_d\bar{g}_{ab}\right), \tag{3.3}$$

where $\bar{g}^{ab}$ is the inverse of $\bar{g}_{ab}$ (see Appendix B). We note that the gauge dependence of the covariant derivative $\bar{\nabla}_a$ appears only through $C^c{}_{ab}$. The Riemann curvature $\bar{R}_{abc}{}^d$ on $\mathcal{M}_\lambda$, which is also pulled back to $\mathcal{M}_0$, is given by [24]:

$$\bar{R}_{abc}{}^d=R_{abc}{}^d-2\nabla_{[a}C^d{}_{b]c}+2C^e{}_{c[a}C^d{}_{b]e}, \tag{3.4}$$

where $R_{abc}{}^d$ is the Riemann curvature on $\mathcal{M}_0$. The perturbative expression for the curvatures are obtained from the expansion of Eq. (3.4) through the expansion of $C^c{}_{ab}$.

The first- and the-second order perturbations of the Riemann, the Ricci, the scalar, the Weyl curvatures, and the Einstein tensors on the general background spacetime are summarized in Ref. [9]. We also derived the perturbative form of the divergence of an arbitrary tensor field of second rank to check the perturbative Bianchi identities in Ref. [9]. In this paper, we only present the perturbative expression for the Einstein tensor, and its derivations in Appendix B.

We expand the Einstein tensor $\bar{G}_a{}^b:=\bar{R}_a{}^b-\frac{1}{2}\delta_a{}^b\bar{R}$ on $\mathcal{M}_\lambda$ as

$$\bar{G}_a{}^b=G_a{}^b+\lambda{}^{(1)}G_a{}^b+\frac{1}{2}\lambda^{2(2)}G_a{}^b+O(\lambda^3). \tag{3.5}$$

As shown in Appendix B, each order perturbation of the Einstein tensor is given by

$$\begin{aligned}{}^{(1)}G_a{}^b &= {}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{H}\right]+\pounds_XG_a{}^b, &(3.6)\\ {}^{(2)}G_a{}^b &= {}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{L}\right]+{}^{(2)}\mathcal{G}_a{}^b\left[\mathcal{H},\mathcal{H}\right]\\ &\quad+2\pounds_X{}^{(1)}\bar{G}_a{}^b+\left\{\pounds_Y-\pounds_X^2\right\}G_a{}^b, &(3.7)\end{aligned}$$

where

$${}^{(1)}\mathcal{G}_a{}^b\left[A\right]:={}^{(1)}\Sigma_a{}^b\left[A\right]-\frac{1}{2}\delta_a{}^{b(1)}\Sigma_c{}^c\left[A\right],\quad {}^{(1)}\Sigma_a{}^b\left[A\right]:=-2\nabla_{[a}H_{d]}{}^{bd}\left[A\right]-A^{cb}R_{ac}, \tag{3.8}$$

$${}^{(2)}\mathcal{G}_a{}^b\left[A,B\right]:={}^{(2)}\Sigma_a{}^b\left[A,B\right]-\frac{1}{2}\delta_a{}^{b(2)}\Sigma_c{}^c\left[A,B\right], \tag{3.9}$$

$$\begin{aligned}{}^{(2)}\Sigma_a{}^b\left[A,B\right] := {}& 2R_{ad}B_c{}^{(b}A^{d)c}+2H_{[a}{}^{de}\left[A\right]H_{d]}{}^b{}_e\left[B\right]+2H_{[a}{}^{de}\left[B\right]H_{d]}{}^b{}_e\left[A\right]\\ &+2A_e{}^d\nabla_{[a}H_{d]}{}^{be}\left[B\right]+2B_e{}^d\nabla_{[a}H_{d]}{}^{be}\left[A\right]+2A_c{}^b\nabla_{[a}H_{d]}{}^{cd}\left[B\right]+2B_c{}^b\nabla_{[a}H_{d]}{}^{cd}\left[A\right],\end{aligned} \tag{3.10}$$

and

$$H_{ab}{}^c\left[A\right]:=\nabla_{(a}A_{b)}{}^c-\frac{1}{2}\nabla^cA_{ab}, \tag{3.11}$$

$$H_{abc}\left[A\right]:=g_{cd}H_{ab}{}^d\left[A\right],\quad H_a{}^{bc}\left[A\right]:=g^{bd}H_{ad}{}^c\left[A\right],\quad H_a{}^b{}_c\left[A\right]:=g_{cd}H_a{}^{bd}\left[A\right]. \tag{3.12}$$

We note that ${}^{(1)}\mathcal{G}_{a}{}^{b}[*]$ and ${}^{(2)}\mathcal{G}_{a}{}^{b}[*,*]$ in Eqs. (3.6) and (3.7) are the gauge invariant parts of the perturbative Einstein tensors, and Eqs. (3.6) and (3.7) have the same forms as Eqs. (2.34) and (2.37), respectively. The expression of ${}^{(2)}\mathcal{G}_{a}{}^{b}[A,B]$ in Eq. (3.9) with Eq. (3.10) is derived by the consideration of the general relativistic gauge-invariant perturbation theory with two infinitesimal parameters in Refs. [8, 9].

We also note that ${}^{(1)}\mathcal{G}_{a}{}^{b}[*]$ and ${}^{(2)}\mathcal{G}_{a}{}^{b}[*,*]$ defined by Eqs. (3.8)–(3.10) satisfy the identities

$$\begin{aligned}
\nabla_{a}{}^{(1)}\mathcal{G}_{b}{}^{a}[A] &= -H_{ca}{}^{a}[A]\,G_{b}{}^{c} + H_{ba}{}^{c}[A]\,G_{c}{}^{a}, &(3.13)\\
\nabla_{a}{}^{(2)}\mathcal{G}_{b}{}^{a}[A,B] &= -H_{ca}{}^{a}[A]\,{}^{(1)}\mathcal{G}_{b}{}^{c}[B] - H_{ca}{}^{a}[B]\,{}^{(1)}\mathcal{G}_{b}{}^{c}[A] + H_{ba}{}^{e}[A]\,{}^{(1)}\mathcal{G}_{e}{}^{a}[B] + H_{ba}{}^{e}[B]\,{}^{(1)}\mathcal{G}_{e}{}^{a}[A]\\
&\quad - \left(H_{bad}[B]\,A^{dc} + H_{bad}[A]\,B^{dc}\right)G_{c}{}^{a} + \left(H_{cad}[B]\,A^{ad} + H_{cad}[A]\,B^{ad}\right)G_{b}{}^{c}, &(3.14)
\end{aligned}$$

for arbitrary tensor fields A_{ab} and B_{ab}, respectively. We can directly confirm these identities without specifying arbitrary tensors A_{ab} and B_{ab} of the second rank, respectively. This implies that our general framework of the second-order gauge invariant perturbation theory discussed here gives a self-consistent formulation of the second-order perturbation theory. These identities (3.13) and (3.14) guarantee the first- and second-order perturbations of the Bianchi identity $\bar{\nabla}_{b}\bar{G}_{a}{}^{b} = 0$ and are also useful when we check whether the derived components of Eqs. (3.8) and (3.9) are correct.

B. Perturbations of the energy momentum tensor and Klein-Gordon equation

Here, we consider the perturbations of the energy momentum tensor of the equation of motion. As a model of the matter field, we only consider the scalar field, for simplicity. Then, equation of motion for a scalar field is the Klein-Gordon equation.

The energy momentum tensor for a scalar field $\bar{\varphi}$ is given by

$$\bar{T}_{a}{}^{b} = \bar{\nabla}_{a}\bar{\varphi}\bar{\nabla}^{b}\bar{\varphi} - \frac{1}{2}\delta_{a}{}^{b}\left(\bar{\nabla}_{c}\bar{\varphi}\bar{\nabla}^{c}\bar{\varphi} + 2V(\bar{\varphi})\right), \quad (3.15)$$

where $V(\bar{\varphi})$ is the potential of the scalar field $\bar{\varphi}$. We expand the scalar field $\bar{\varphi}$ as

$$\bar{\varphi} = \varphi + \lambda\hat{\varphi}_{1} + \frac{1}{2}\lambda^{2}\hat{\varphi}_{2} + O(\lambda^{3}), \quad (3.16)$$

where φ is the background value of the scalar field $\bar{\varphi}$. Further, following to the decomposition formulae (2.34) and (2.35), each order perturbation of the scalar field $\bar{\varphi}$ is decomposed as

$$\begin{aligned}
\hat{\varphi}_{1} &=: \varphi_{1} + \pounds_{X}\varphi, &(3.17)\\
\hat{\varphi}_{2} &=: \varphi_{2} + 2\pounds_{X}\hat{\varphi}_{1} + \left(\pounds_{Y} - \pounds_{X}^{2}\right)\varphi, &(3.18)
\end{aligned}$$

where φ_{1} and φ_{2} are the first- and the second-order gauge-invariant perturbations of the scalar field, respectively.

Through the perturbative expansions (3.16) and (B2) of the scalar field $\bar{\varphi}$ and the inverse metric, the energy momentum tensor (3.15) is also expanded as

$$\bar{T}_{a}{}^{b} = T_{a}{}^{b} + \lambda^{(1)}\left(T_{a}{}^{b}\right) + \frac{1}{2}\lambda^{2\,(2)}\left(T_{a}{}^{b}\right) + O(\lambda^{3}). \quad (3.19)$$

The background energy momentum tensor $T_{a}{}^{b}$ is given by the replacement $\bar{\varphi} \to \varphi$ in Eq. (3.15). Further, through the decompositions (2.23), (2.32), (3.17), and (3.18), the perturbations of the energy momentum tensor ${}^{(1)}\left(T_{a}{}^{b}\right)$ and ${}^{(2)}\left(T_{a}{}^{b}\right)$ are also decomposed as

$$\begin{aligned}
{}^{(1)}\left(T_{a}{}^{b}\right) &=: {}^{(1)}\mathcal{T}_{a}{}^{b} + \pounds_{X}T_{a}{}^{b}, &(3.20)\\
{}^{(2)}\left(T_{a}{}^{b}\right) &=: {}^{(2)}\mathcal{T}_{a}{}^{b} + 2\pounds_{X}{}^{(1)}\left(T_{a}{}^{b}\right)\\
&\qquad + \left(\pounds_{Y} - \pounds_{X}^{2}\right)T_{a}{}^{b}, &(3.21)
\end{aligned}$$

where the gauge-invariant parts ${}^{(1)}\mathcal{T}_{a}{}^{b}$ and ${}^{(2)}\mathcal{T}_{a}{}^{b}$ of the first and the second order are given by

$$\begin{aligned}
{}^{(1)}\mathcal{T}_{a}{}^{b} &:= \nabla_{a}\varphi\nabla^{b}\varphi_{1} - \nabla_{a}\varphi\mathcal{H}^{bc}\nabla_{c}\varphi + \nabla_{a}\varphi_{1}\nabla^{b}\varphi - \delta_{a}{}^{b}\left(\nabla_{c}\varphi\nabla^{c}\varphi_{1} - \frac{1}{2}\nabla_{c}\varphi\mathcal{H}^{dc}\nabla_{d}\varphi + \varphi_{1}\frac{\partial V}{\partial\varphi}\right), &(3.22)\\
{}^{(2)}\mathcal{T}_{a}{}^{b} &:= \nabla_{a}\varphi\nabla^{b}\varphi_{2} + \nabla_{a}\varphi_{2}\nabla^{b}\varphi - \nabla_{a}\varphi g^{bd}\mathcal{L}_{dc}\nabla^{c}\varphi - 2\nabla_{a}\varphi\mathcal{H}^{bc}\nabla_{c}\varphi_{1} + 2\nabla_{a}\varphi\mathcal{H}^{bd}\mathcal{H}_{dc}\nabla^{c}\varphi + 2\nabla_{a}\varphi_{1}\nabla^{b}\varphi_{1}\\
&\qquad -2\nabla_{a}\varphi_{1}\mathcal{H}^{bc}\nabla_{c}\varphi - \delta_{a}{}^{b}\left(\nabla_{c}\varphi\nabla^{c}\varphi_{2} - \frac{1}{2}\nabla^{c}\varphi\mathcal{L}_{dc}\nabla^{d}\varphi + \nabla^{c}\varphi\mathcal{H}^{de}\mathcal{H}_{ec}\nabla_{d}\varphi - 2\nabla_{c}\varphi\mathcal{H}^{dc}\nabla_{d}\varphi_{1}\right.\\
&\qquad\qquad \left. + \nabla_{c}\varphi_{1}\nabla^{c}\varphi_{1} + \varphi_{2}\frac{\partial V}{\partial\varphi} + \varphi_{1}^{2}\frac{\partial^{2}V}{\partial\varphi^{2}}\right). &(3.23)
\end{aligned}$$

We note that Eq. (3.20) and (3.21) have the same form as (2.36) and (2.37), respectively.

Next, we consider the perturbation of the Klein-Gordon equation

$$\bar{C}_{(K)} := \bar{\nabla}^a\bar{\nabla}_a\bar{\varphi} - \frac{\partial V}{\partial\bar{\varphi}}(\bar{\varphi}) = 0. \tag{3.24}$$

Through the perturbative expansions (3.16) and (2.22), the Klein-Gordon equation (3.24) is expanded as

$$\bar{C}_{(K)} =: C_{(K)} + \lambda \stackrel{(1)}{C}_{(K)} + \frac{1}{2}\lambda^2 \stackrel{(2)}{C}_{(K)} + O(\lambda^3). \tag{3.25}$$

$C_{(K)}$ is the background Klein-Gordon equation

$$C_{(K)} \;:=\; \nabla_a\nabla^a\varphi - \frac{\partial V}{\partial\bar{\varphi}}(\varphi) = 0. \tag{3.26}$$

The first- and the second-order perturbations $\stackrel{(1)}{C}_{(K)}$ and $\stackrel{(2)}{C}_{(K)}$ are also decomposed into the gauge-invariant and the gauge-variant parts as

$$\stackrel{(1)}{C}_{(K)} =: \stackrel{(1)}{\mathcal{C}}_{(K)} + \pounds_X C_{(K)}, \quad \stackrel{(2)}{C}_{(K)} =: \stackrel{(2)}{\mathcal{C}}_{(K)} + 2\pounds_X \stackrel{(1)}{C}_{(K)} + \left(\pounds_Y - \pounds_X^2\right) C_{(K)}, \tag{3.27}$$

where

$$\stackrel{(1)}{\mathcal{C}}_{(K)} \;:=\; \nabla^a\nabla_a\varphi_1 - H_a{}^{ac}[\mathcal{H}]\nabla_c\varphi - \mathcal{H}^{ab}\nabla_a\nabla_b\varphi - \varphi_1\frac{\partial^2 V}{\partial\bar{\varphi}^2}(\varphi), \tag{3.28}$$

$$\begin{aligned}\stackrel{(2)}{\mathcal{C}}_{(K)} \;:=\;& \nabla^a\nabla_a\varphi_2 - H_a{}^{ac}[\mathcal{L}]\nabla_c\varphi + 2H_a{}^{ad}[\mathcal{H}]\mathcal{H}_{cd}\nabla^c\varphi - 2H_a{}^{ac}[\mathcal{H}]\nabla_c\varphi_1 + 2\mathcal{H}^{ab}H_{ab}{}^c[\mathcal{H}]\nabla_c\varphi \\ &-\mathcal{L}^{ab}\nabla_a\nabla_b\varphi + 2\mathcal{H}^a{}_d\mathcal{H}^{db}\nabla_a\nabla_b\varphi - 2\mathcal{H}^{ab}\nabla_a\nabla_b\varphi_1 - \varphi_2\frac{\partial^2 V}{\partial\bar{\varphi}^2}(\varphi) - (\varphi_1)^2\frac{\partial^3 V}{\partial\bar{\varphi}^3}(\varphi).\end{aligned} \tag{3.29}$$

Here, we note that Eqs. (3.27) have the same form as Eqs. (2.36) and (2.37).

By virtue of the order by order evaluations of the Klein-Gordon equation, the first- and the second-order perturbation of the Klein-Gordon equation are necessarily given in gauge-invariant form as

$$\stackrel{(1)}{\mathcal{C}}_{(K)} = 0, \quad \stackrel{(2)}{\mathcal{C}}_{(K)} = 0. \tag{3.30}$$

We should note that, in Ref. [12], we summarized the formulae of the energy momentum tensors for an perfect fluid, an imperfect fluid, and a scalar field. Further, we also summarized the equations of motion of these three matter fields: i.e., the energy continuity equation and the Euler equation for a perfect fluid; the energy continuity equation and the Navier-Stokes equation for an imperfect fluid; the Klein-Gordon equation for a scalar field. All these formulae also have the same form as the decomposition formulae (2.36) and (2.37). In this sense, we may say that the decomposition formulae (2.36) and (2.37) are universal.

C. Perturbations of the Einstein equation

Finally, we impose the perturbed Einstein equation of each order,

$${}^{(1)}G_a{}^b = 8\pi G \;\; {}^{(1)}T_a{}^b, \quad {}^{(2)}G_a{}^b = 8\pi G \;\; {}^{(2)}T_a{}^b. \tag{3.31}$$

Then, the perturbative Einstein equation is given by

$${}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{H}\right] \;=\; 8\pi G {}^{(1)}\mathcal{T}_a{}^b \tag{3.32}$$

at linear order and

$${}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{L}\right] + {}^{(2)}\mathcal{G}_a{}^b\left[\mathcal{H},\mathcal{H}\right] \;=\; 8\pi G \;\; {}^{(2)}\mathcal{T}_a{}^b \tag{3.33}$$

at second order. These explicitly show that, order by order, the Einstein equations are necessarily given in terms of gauge invariant variables only.

Together with Eqs. (3.30), we have seen that the first- and the second-order perturbations of the Einstein equations and the Klein-Gordon equation are necessarily given in gauge-invariant form. This implies that we do not have to consider the gauge degree of freedom, at least in the level where we concentrate only on the equations of the system.

We have reviewed the general outline of the second-order gauge invariant perturbation theory. We also note that the ingredients of this section are independent of the explicit form of the background metric g_{ab}, except for the decomposition assumption (2.23) for the linear-order metric perturbations and are valid not only in cosmological perturbation case but also the other generic situations if Eq. (2.23) is correct. Within this general framework, we develop a second-order cosmological perturbation theory in terms of the gauge invariant variables.

IV. COSMOLOGICAL BACKGROUND SPACETIME AND EQUATIONS

The background spacetime $\mathcal{M}_0$ considered in cosmological perturbation theory is a homogeneous, isotropic universe that is foliated by the three-dimensional hypersurface $\Sigma(\eta)$, which is parametrized by η. Each hypersurface of $\Sigma(\eta)$ is a maximally symmetric three-space[25], and the spacetime metric of this universe is given by

$$g_{ab} = a^2(\eta)\left(-(d\eta)_a(d\eta)_b + \gamma_{ij}(dx^i)_a(dx^j)_b\right), \quad (4.1)$$

where $a = a(\eta)$ is the scale factor, γ_{ij} is the metric on the maximally symmetric 3-space with curvature constant K, and the indices $i, j, k, ...$ for the spatial components run from 1 to 3.

To study the Einstein equation for this background spacetime, we introduce the energy-momentum tensor for a scalar field, which is given by

$$\begin{aligned} T_a{}^b &= \nabla_a\varphi\nabla^b\varphi - \frac{1}{2}\delta_a{}^b\left(\nabla_c\varphi\nabla^c\varphi + 2V(\varphi)\right) \quad (4.2)\\ &= -\left(\frac{1}{2a^2}(\partial_\eta\varphi)^2 + V(\varphi)\right)(d\eta)_a\left(\frac{\partial}{\partial\eta}\right)^b \\ &\quad + \left(\frac{1}{2a^2}(\partial_\eta\varphi)^2 - V(\varphi)\right)\gamma_a{}^b, \quad (4.3)\end{aligned}$$

where we assumed that the scalar field φ is homogeneous

$$\varphi = \varphi(\eta) \quad (4.4)$$

and $\gamma_a{}^b$ are defined as

$$\gamma_{ab} := \gamma_{ij}(dx^i)_a(dx^j)_b, \quad \gamma_a{}^b := \gamma_i{}^j(dx^i)_a(\partial/\partial x^j)^b. (4.5)$$

The background Einstein equations $G_a{}^b = 8\pi G T_a{}^b$ for this background spacetime filled with the single scalar field are given by

$$\mathcal{H}^2 + K = \frac{8\pi G}{3}a^2\left(\frac{1}{2a^2}(\partial_\eta\varphi)^2 + V(\varphi)\right), \quad (4.6)$$

$$2\partial_\eta\mathcal{H} + \mathcal{H}^2 + K = 8\pi G\left(-\frac{1}{2}(\partial_\eta\varphi)^2 + a^2V(\varphi)\right). \quad (4.7)$$

We also note that the equations (4.6) and (4.7) lead to

$$\mathcal{H}^2 + K - \partial_\eta\mathcal{H} = 4\pi G(\partial_\eta\varphi)^2. \quad (4.8)$$

Equation (4.8) is also useful when we derive the perturbative Einstein equations.

Next, we consider the background Klein-Gordon equation which is the equation of motion $\nabla_a T_b{}^a = 0$ for the scalar field

$$\partial_\eta^2\varphi + 2\mathcal{H}\partial_\eta\varphi + a^2\frac{\partial V}{\partial\varphi} = 0. \quad (4.9)$$

The Klein-Gordon equation (4.9) is also derived from the Einstein equations (4.6) and (4.7). This is a well known fact and is just due to the Bianchi identity of the background spacetime. However, these types of relation are useful to check whether the derived system of equations is consistent.

V. EQUATIONS FOR THE FIRST-ORDER COSMOLOGICAL PERTURBATIONS

On the cosmological background spacetime in the last section, we develop the perturbation theory in the gauge-invariant manner. In this section, we summarize the first-order perturbation of the Einstein equation and the Klein-Gordon equations. In Sec. V A, we show that the assumption on the decomposition (2.23) of the linear-order metric perturbation is correct. In Sec. V B, we summarize the first-order perturbation of the Einstein equation. Finally, in Sec. V C, we show the first-order perturbation of the Klein-Gordon equation.

A. Gauge-invariant metric perturbations

Here, we consider the first-order metric perturbation h_{ab} and show the assumption on the decomposition (2.23) is correct in the background metric Eq. (4.1). To accomplish the decomposition (2.23), first, we assume the existence of the Green functions $\Delta^{-1} := (D^iD_i)^{-1}$, $(\Delta + 2K)^{-1}$, and $(\Delta + 3K)^{-1}$, where D_i is the covariant derivative associated with the metric γ_{ij} and K is the curvature constant of the maximally symmetric three space. Next, we consider the decomposition of the linear-order metric perturbation h_{ab} as

$$\begin{aligned} h_{ab} &= h_{\eta\eta}(d\eta)_a(d\eta)_b \\ &\quad + 2\left(D_ih_{(VL)} + h_{(V)i}\right)(d\eta)_{(a}(dx^i)_{b)} \quad (5.1)\\ &\quad + a^2\left\{h_{(L)}\gamma_{ij} + \left(D_iD_j - \frac{1}{3}\gamma_{ij}\Delta\right)h_{(TL)}\right. \\ &\qquad \left. + 2D_{(i}h_{(TV)j)} + h_{(TT)ij}\right\}(dx^i)_a(dx^j)_b,\end{aligned}$$

where $h_{(V)i}$, $h_{(TV)j}$, and $h_{(TT)ij}$ satisfy the properties

$$\begin{aligned} &D^ih_{(V)i} = 0, \quad D^ih_{(TV)i} = 0, \\ &h_{(TT)ij} = h_{(TT)ji}, \quad h_{(T)}{}^i{}_i := \gamma^{ij}h_{(T)ij} = 0, (5.2)\\ &D^ih_{(TT)ij} = 0.\end{aligned}$$

The gauge-transformation rules for the variables $h_{\eta\eta}$, $h_{(VL)}$, $h_{(V)i}$, $h_{(L)}$, $h_{(TL)}$, $h_{(TV)j}$ and $h_{(TT)ij}$ are derived from Eq. (2.25). Inspecting these gauge-transformation rules, we define the gauge-variant part X_a in Eq. (2.23):

$$\begin{aligned} X_a &:= \left(h_{(VL)} - \frac{1}{2}a^2\partial_\eta h_{(TL)}\right)(d\eta)_a \\ &\quad + a^2\left(h_{(TV)i} + \frac{1}{2}D_ih_{(TL)}\right)(dx^i)_a. \quad (5.3)\end{aligned}$$

We can easily check this vector field X_a satisfies Eq. (2.24). Subtracting gauge variant-part $\pounds_X g_{ab}$ from h_{ab}, we have the gauge-invariant part $\mathcal{H}_{ab}$ in Eq. (2.23):

$$\begin{aligned} \mathcal{H}_{ab} &= a^2\left\{-2\stackrel{(1)}{\Phi}(d\eta)_a(d\eta)_b + 2\stackrel{(1)}{\nu}_i(d\eta)_{(a}(dx^i)_{b)}\right. \\ &\qquad \left. + \left(-2\stackrel{(1)}{\Psi}\gamma_{ij} + \stackrel{(1)}{\chi}_{ij}\right)(dx^i)_a(dx^j)_b\right\}, \quad (5.4)\end{aligned}$$

where the properties $D^i \stackrel{(1)}{\nu}_i := \gamma^{ij} D_i \stackrel{(1)}{\nu}_j = \stackrel{(1)}{\chi_i}{}^i := \gamma^{ij} \stackrel{(1)}{\chi_{ij}} = D^i \stackrel{(1)}{\chi}_{ij} = 0$ are satisfied as consequences of Eqs. (5.2).

Thus, we may say that our assumption for the decomposition (2.23) in linear-order metric perturbation is correct in the case of cosmological perturbations. However, we have to note that to accomplish Eq. (2.23), we assumed the existence of the Green functions Δ^{-1}, $(\Delta + 2K)^{-1}$, and $(\Delta + 3K)^{-1}$. As shown in Ref. [11], this assumption is necessary to guarantee the one to one correspondence between the variables $\{h_{\eta\eta}, h_{i\eta}, h_{ij}\}$ and $\{h_{\eta\eta}, h_{(VL)}, h_{(V)i}, h_{(L)}, h_{(TL)}, h_{(TV)j}, h_{(TT)ij}\}$, but excludes some perturbative modes of the metric perturbations which belong to the kernel of the operator Δ, $(\Delta + 2K)$, and $(\Delta + 3K)$ from our consideration. For example, homogeneous modes belong to the kernel of the operator Δ and are excluded from our consideration. If we have to treat these modes, the separate treatments are necessary. In this paper, we ignore these modes, for simplicity.

We also note the fact that the definition (2.23) of the gauge-invariant variables is not unique. This comes from the fact that we can always construct new gauge-invariant quantities by the combination of the gauge-invariant variables. For example, using the gauge-invariant variables $\stackrel{(1)}{\Phi}$ and $\stackrel{(1)}{\nu_i}$ of the first-order metric perturbation, we can define a vector field Z_a by $Z_a := -a \stackrel{(1)}{\Phi} (d\eta)_a + a \stackrel{(1)}{\nu_i} (dx^i)_a$ which is gauge-invariant. Then, we can rewrite the decomposition formula (2.23) for the linear-order metric perturbation as

$$\begin{aligned} h_{ab} &= \mathcal{H}_{ab} - \pounds_Z g_{ab} + \pounds_Z g_{ab} + \pounds_X g_{ab}, \\ &=: \mathcal{K}_{ab} + \pounds_{X+Z} g_{ab}, \end{aligned} \tag{5.5}$$

where we have defined new gauge-invariant variable $\mathcal{K}_{ab}$ by $\mathcal{K}_{ab} := \mathcal{H}_{ab} - \pounds_Z g_{ab}$. Clearly, $\mathcal{K}_{ab}$ is gauge-invariant and the vector field $X^a + Z^a$ satisfies Eq. (2.24). In spite of this non-uniqueness, we specify the components of the tensor $\mathcal{H}_{ab}$ as Eq. (5.4), which is the gauge-invariant part of the linear-order metric perturbation associated with the longitudinal gauge.

The non-uniqueness of the definitions of gauge-invariant variables is related to the "gauge-fixing" for the linear-order metric perturbations. Due to this non-uniqueness, we can consider the gauge-fixing in the first-order metric perturbation from two different points of view. The first point of view is that the gauge-fixing is to specify the gauge-variant part X^a. For example, the longitudinal gauge is realized by the gauge fixing $X^a = 0$. Due to this gauge fixing $X^a = 0$, we can regard the fact that perturbative variables in the longitudinal gauge are the completely gauge fixed variables. On the other hand, we may also regard that the gauge fixing is the specification of the gauge-invariant vector field Z^a in Eq. (5.5). In this point of view, we do not specify the vector field X^a. Instead, we have to specify the gauge-invariant vector Z^a or equivalently to specify the gauge-invariant metric perturbation $\mathcal{K}_{ab}$ without specifying X^a so that the first-order metric perturbation h_{ab} coincides with the gauge-invariant variables $\mathcal{K}_{ab}$ when we fix the gauge X^a so that $X^a + Z^a = 0$. These two different point of view of "gauge fixing" is equivalent with each other due to the non-uniqueness of the definition (5.5) of the gauge-invariant variables.

B. First-order Einstein equations

Here, we derive the linear-order Einstein equation (3.32). To derive the components of the gauge invariant part of the linearized Einstein tensor ${}^{(1)}\mathcal{G}_a{}^b[\mathcal{H}]$, which is defined by Eqs. (3.8), we first derive the components of the tensor $H_{ab}{}^c[\mathcal{H}]$, which is defined in Eq. (3.11) with $A_{ab} = \mathcal{H}_{ab}$ and its component (5.4). These components are summarized in Ref. [11].

From Eq. (3.8), the component of ${}^{(1)}\mathcal{G}_a{}^b[\mathcal{H}]$ are summarized as

$$ {}^{(1)}\mathcal{G}_\eta{}^\eta[\mathcal{H}] = -\frac{1}{a^2}\left\{(-6\mathcal{H}\partial_\eta + 2\Delta + 6K)\stackrel{(1)}{\Psi} - 6\mathcal{H}^2 \stackrel{(1)}{\Phi}\right\}, \tag{5.6}$$

$$ {}^{(1)}\mathcal{G}_i{}^\eta[\mathcal{H}] = -\frac{1}{a^2}\left(2\partial_\eta D_i \stackrel{(1)}{\Psi} + 2\mathcal{H} D_i \stackrel{(1)}{\Phi} - \frac{1}{2}(\Delta + 2K)\stackrel{(1)}{\nu_i}\right), \tag{5.7}$$

$$ {}^{(1)}\mathcal{G}_\eta{}^i[\mathcal{H}] = \frac{1}{a^2}\left\{2\partial_\eta D^i \stackrel{(1)}{\Psi} + 2\mathcal{H} D^i \stackrel{(1)}{\Phi} + \frac{1}{2}\left(-\Delta + 2K + 4\mathcal{H}^2 - 4\partial_\eta\mathcal{H}\right)\stackrel{(1)}{\nu^i}\right\}, \tag{5.8}$$

$$\begin{aligned} {}^{(1)}\mathcal{G}_i{}^j[\mathcal{H}] = \frac{1}{a^2}\Bigg[& D_i D^j\left(\stackrel{(1)}{\Psi} - \stackrel{(1)}{\Phi}\right) + \left\{\left(-\Delta + 2\partial_\eta^2 + 4\mathcal{H}\partial_\eta - 2K\right)\stackrel{(1)}{\Psi} + \left(2\mathcal{H}\partial_\eta + 4\partial_\eta\mathcal{H} + 2\mathcal{H}^2 + \Delta\right)\stackrel{(1)}{\Phi}\right\}\gamma_i{}^j \\ & -\frac{1}{2a^2}\partial_\eta\left\{a^2\left(D_i \stackrel{(1)}{\nu^j} + D^j \stackrel{(1)}{\nu_i}\right)\right\} + \frac{1}{2}\left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta\right)\stackrel{(1)}{\chi_i}{}^j\Bigg]. \end{aligned} \tag{5.9}$$

Straightforward calculations show that these components of the first-order gauge invariant perturbation ${}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{H}\right]$ of the Einstein tensor satisfies the identity (3.13). Although this confirmation is also possible without specification of the tensor $\mathcal{H}_{ab}$, the confirmation of Eq. (3.13) through the explicit components (5.6)–(5.9) implies that we have derived the components of ${}^{(1)}\mathcal{G}_a{}^b\left[\mathcal{H}\right]$ consistently.

Next, we summarize the first-order perturbation of the energy momentum tensor for a scalar field. Since, at the background level, we assume that the scalar field φ is homogeneous as Eq. (4.4), the components of the gauge-invariant part of the first-order energy-momentum tensor ${}^{(1)}\mathcal{T}_a{}^b$ are given by

$$ {}^{(1)}\mathcal{T}_\eta{}^\eta = -\frac{1}{a^2}\left(\partial_\eta\varphi_1\partial_\eta\varphi - \stackrel{(1)}{\Phi}(\partial_\eta\varphi)^2 + a^2\frac{dV}{d\varphi}\varphi_1\right), \quad {}^{(1)}\mathcal{T}_i{}^\eta = -\frac{1}{a^2}D_i\varphi_1\partial_\eta\varphi, \tag{5.10} $$

$$ {}^{(1)}\mathcal{T}_\eta{}^i = \frac{1}{a^2}\partial_\eta\varphi\left(D^i\varphi_1 + (\partial_\eta\varphi)\stackrel{(1)}{\nu^i}\right), \quad {}^{(1)}\mathcal{T}_i{}^j = \frac{1}{a^2}\gamma_i{}^j\left(\partial_\eta\varphi_1\partial_\eta\varphi - \stackrel{(1)}{\Phi}(\partial_\eta\varphi)^2 - a^2\frac{dV}{d\varphi}\varphi_1\right). \tag{5.11} $$

The second equation in (5.11) shows that there is no anisotropic stress in the energy-momentum tensor of the single scalar field. Then, we obtain

$$ \stackrel{(1)}{\Phi} = \stackrel{(1)}{\Psi}. \tag{5.12} $$

From Eqs. (5.6)–(5.11) and (5.12), the components of scalar parts of the linearized Einstein equation (3.32) are given as[3]

$$ \begin{aligned} &\left(\Delta - 3\mathcal{H}\partial_\eta + 4K - \partial_\eta\mathcal{H} - 2\mathcal{H}^2\right)\stackrel{(1)}{\Phi} \\ &\qquad = 4\pi G\left(\partial_\eta\varphi_1\partial_\eta\varphi + a^2\frac{dV}{d\varphi}\varphi_1\right), \end{aligned} \tag{5.13} $$

$$ \partial_\eta\stackrel{(1)}{\Phi} + \mathcal{H}\stackrel{(1)}{\Phi} = 4\pi G\varphi_1\partial_\eta\varphi, \tag{5.14} $$

$$ \begin{aligned} &\left(\partial_\eta^2 + 3\mathcal{H}\partial_\eta + \partial_\eta\mathcal{H} + 2\mathcal{H}^2\right)\stackrel{(1)}{\Phi} \\ &\qquad = 4\pi G\left(\partial_\eta\varphi_1\partial_\eta\varphi - a^2\frac{dV}{d\varphi}\varphi_1\right). \end{aligned} \tag{5.15} $$

In the derivation of Eqs. (5.13)–(5.15), we have used Eq. (4.8). We also note that only two of these equations are independent. Further, the vector part of the component ${}^{(1)}\mathcal{G}_i{}^\eta\left[\mathcal{H}\right] = 8\pi G{}^{(1)}\mathcal{T}_i{}^\eta$ shows that

$$ \stackrel{(1)}{\nu}_i = 0. \tag{5.16} $$

The equation for the tensor mode $\stackrel{(1)}{\chi}_{ij}$ is given by

$$ \left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta\right)\stackrel{(1)}{\chi}_i{}^j = 0. \tag{5.17} $$

Combining Eqs. (5.13) and (5.15), we eliminate the potential term of the scalar field and thereby obtain

$$ \left(\partial_\eta^2 + \Delta + 4K\right)\stackrel{(1)}{\Phi} = 8\pi G\partial_\eta\varphi_1\partial_\eta\varphi. \tag{5.18} $$

Further, using Eq. (5.14) to express $\partial_\eta\varphi_1$ in terms of $\partial_\eta\stackrel{(1)}{\Phi}$ and $\stackrel{(1)}{\Phi}$, we also eliminate $\partial_\eta\varphi_1$ in Eq. (5.18). Hence, we have

$$ \left\{\partial_\eta^2 + 2\left(\mathcal{H} - \frac{2\partial_\eta^2\varphi}{\partial_\eta\varphi}\right)\partial_\eta - \Delta - 4K + 2\left(\partial_\eta\mathcal{H} - \frac{\mathcal{H}\partial_\eta^2\varphi}{\partial_\eta\varphi}\right)\right\}\stackrel{(1)}{\Phi} = 0. \tag{5.19} $$

This is the master equation for the scalar mode perturbation of the cosmological perturbation in universe filled with a single scalar field. It is also known that Eq. (5.19) reduces to a simple equation through a change of variables [3].

C. First-order Klein-Gordon equations

Next, we consider the first-order perturbation of the Klein-Gordon equation (3.28). By the straightforward calculations using Eqs. (4.1), (5.4), (4.4), (4.9), and the components $H_a{}^{ac}$ summarized in Ref. [11], the gauge-invariant part $\stackrel{(1)}{\mathcal{C}}_{(K)}$ of the first-order Klein-Gordon equa-

tion defined by Eq. (3.28) is given by

$$\begin{aligned} -a^2 \overset{(1)}{\mathcal{C}}_{(K)} &= \partial_\eta^2\varphi_1 + 2\mathcal{H}\partial_\eta\varphi_1 - \Delta\varphi_1 \\ &\quad - \left(\partial_\eta \overset{(1)}{\Phi} + 3\partial_\eta \overset{(1)}{\Psi}\right)\partial_\eta\varphi \\ &\quad + 2a^2 \overset{(1)}{\Phi} \frac{\partial V}{\partial\bar{\varphi}}(\varphi) + a^2\varphi_1 \frac{\partial^2 V}{\partial\bar{\varphi}^2}(\varphi) \\ &= 0. \end{aligned} \tag{5.20}$$

Through the background Einstein equations (4.6), (4.7), and the first-order perturbations (5.14) and (5.19) of the Einstein equation, we can easily derive the first-order perturbation of the Klein-Gordon equation (5.20)[13]. Hence, the first-order perturbation of the Klein-Gordon equation is not independent of the background and the first-order perturbation of the Einstein equation. Therefore, from the viewpoint of the Cauchy problem, any information obtained from the first-order perturbation of the Klein-Gordon equation should also be obtained from the set of the background and the first-order the Einstein equation, in principle.

VI. EQUATIONS FOR THE SECOND-ORDER COSMOLOGICAL PERTURBATIONS

Now, we develop the second-order perturbation theory on the cosmological background spacetime in Sec. IV within the general framework of the gauge-invariant perturbation theory reviewed in Sec. II. Since we have already confirm the important step of our general framework, i.e., the assumption for the decomposition (2.23) of the linear-order metric perturbation is correct. Hence, the general framework reviewed in Sec. II is applicable. Applying this framework, we define the second-order gauge invariant variables of the metric perturbation in Sec. VI A. In Sec. VI B, we summarize the explicit components of the gauge invariant parts of the second-order perturbation of the Einstein tensor. In Sec. VI C, we summarize the explicit components of the second-order perturbation of the energy-momentum tensor and the Klein-Gordon equations. Then, in Sec. VI D, we derive the second-order Einstein equations in terms of gauge-invariant variables. The resulting equations have the source terms which constitute of the quadratic terms of the linear-order perturbations. Although these source terms have complicated forms, we give identities which comes from the consistency of all the second-order perturbations of the Einstein equation and the Klein-Gordon equation in Sec. VI E.

A. Gauge-invariant metric perturbations

First, we consider the components of the gauge invariant variables for the metric perturbation of second order. The variable $\hat{L}_{ab}$ defined by Eq. (2.27) is transformed as Eq. (2.28) under the gauge transformation and we may regard the generator σ_a defined by Eq. (2.29) as an arbitrary vector field on $\mathcal{M}_0$ from the fact that the generator ξ_2^a in Eq. (2.29) is arbitrary. We can apply the procedure to find gauge invariant variables for the first-order metric perturbations (5.4) in Sec. V A. Then, we can accomplish the decomposition (2.30). Following to the same argument as in the linear case, we may choose the components of the gauge invariant variables $\mathcal{L}_{ab}$ in Eq. (2.32) as

$$\begin{aligned} \mathcal{L}_{ab} &= -2a^2 \overset{(2)}{\Phi} (d\eta)_a(d\eta)_b + 2a^2 \overset{(2)}{\nu_i} (d\eta)_{(a}(dx^i)_{b)} \\ &\quad + a^2\left(-2\overset{(2)}{\Psi}\gamma_{ij} + \overset{(2)}{\chi_{ij}}\right)(dx^i)_a(dx^j)_b, \end{aligned} \tag{6.1}$$

where $\overset{(2)}{\nu}{}_i$ and $\overset{(2)}{\chi_{ij}}$ satisfy the equations

$$D^i \overset{(2)}{\nu_i} = 0, \quad \overset{(2)}{\chi}{}^i{}_i = 0, \quad D^i \overset{(2)}{\chi_{ij}} = 0. \tag{6.2}$$

The gauge invariant variables $\overset{(2)}{\Phi}$ and $\overset{(2)}{\Psi}$ are the scalar mode perturbations of second order, and $\overset{(2)}{\nu_i}$ and $\overset{(2)}{\chi_{ij}}$ are the second-order vector and tensor modes of the metric perturbations, respectively.

Here, we also note the fact that the decomposition (2.32) is not unique. This situation is similar to the case of the linear-order, but more complicated. In the definition of the gauge invariant variables of the second-order metric perturbation, we may replace

$$X^a = X'^a - Z'^a, \tag{6.3}$$

where Z'^a is gauge invariant and X'^a is transformed as

$${}_{\mathcal{Y}}X'^a - {}_{\mathcal{X}}X'^a = \xi_1^a \tag{6.4}$$

under the gauge transformation $\mathcal{X}_\lambda \to \mathcal{Y}_\lambda$. This Z'^a may be different from the vector Z^a in Eq. (5.5). By the replacement (6.3), the second-order metric perturbation (2.32) is given in the form

$$l_{ab} =: \mathcal{J}_{ab} + 2\pounds_{X'}h_{ab} + \left(\pounds_{Y'} - \pounds_{X'}^2\right)g_{ab}, \tag{6.5}$$

where we defined

$$\begin{aligned} \mathcal{J}_{ab} &:= \mathcal{L}_{ab} - \pounds_W g_{ab} - 2\pounds_{Z'}\mathcal{K}_{ab} \\ &\quad -2\pounds_{Z'}\pounds_Z g_{ab} + \pounds_{Z'}^2 g_{ab}, \end{aligned} \tag{6.6}$$

$$Y'^a := Y^a + W^a + [X', Z']^a. \tag{6.7}$$

Here, the vector field W^a in Eq. (6.7) constitute of some components of gauge invariant second-order metric perturbation $\mathcal{L}_{ab}$ like Z^a in Eq. (5.5). The tensor field $\mathcal{J}_{ab}$ is manifestly gauge invariant. The gauge transformation rule of the new gauge-variant part Y'^a of the second-order metric perturbation is given by

$${}_{\mathcal{Y}}Y'^a - {}_{\mathcal{X}}Y'^a = \xi_{(2)}^a + [\xi_{(1)}, X']^a. \tag{6.8}$$

Although Eq. (6.5) is similar to Eq. (2.32), the tensor fields $\mathcal{L}_{ab}$ and $\mathcal{J}_{ab}$ are different from each other. Thus, the definition of the gauge invariant variables for the second-order metric perturbation is not unique in a more complicated way than the linear order. This non-uniqueness of gauge-invariant variables for the metric perturbations propagates to the definition (2.34) and (2.35) of the gauge invariant variables for matter fields.

In spite of the existence of infinitely many definitions of the gauge invariant variables, in this paper, we consider the components of $\mathcal{L}_{ab}$ given by Eq. (6.1). Eq. (6.1) corresponds to the second-order extension of the longitudinal gauge, which is called Poisson gauge $X^a = Y^a = 0$.

B. Einstein tensor

Here, we evaluate the second-order perturbation of the Einstein tensor (3.7) with the cosmological background (4.1). We evaluate the term ${}^{(1)}\mathcal{G}_{a}{}^{b}[\mathcal{L}]$ and ${}^{(2)}\mathcal{G}_{a}{}^{b}[\mathcal{H},\mathcal{H}]$ in the Einstein equation (3.33).

First, we evaluate the term ${}^{(1)}\mathcal{G}_{a}{}^{b}[\mathcal{L}]$ in the Einstein equation (3.33). Because the components (6.1) of $\mathcal{L}_{ab}$ are obtained through the replacements

$$\stackrel{(1)}{\Phi} \to \stackrel{(2)}{\Phi}, \quad \stackrel{(1)}{\nu}_{i} \to \stackrel{(2)}{\nu}_{i}, \quad \stackrel{(1)}{\Psi} \to \stackrel{(2)}{\Psi}, \quad \stackrel{(1)}{\chi}_{ij} \to \stackrel{(2)}{\chi}_{ij} \tag{6.9}$$

in the components (5.4) of $\mathcal{H}_{ab}$, we easily obtain the components of ${}^{(1)}\mathcal{G}_{a}{}^{b}[\mathcal{L}]$ through the replacements (6.9) in Eqs. (5.6)–(5.9).

From Eq. (5.4), we can derive the components of ${}^{(2)}\mathcal{G}_{a}{}^{b} = {}^{(2)}\mathcal{G}_{a}{}^{b}[\mathcal{H},\mathcal{H}]$ defined by Eqs. (3.9)–(3.12) in a straightforward manner. Here, we use the results (5.12) and (5.16) of the first-order Einstein equations, for simplicity. Then the explicit components ${}^{(2)}\mathcal{G}_{a}{}^{b} = {}^{(2)}\mathcal{G}_{a}{}^{b}[\mathcal{H},\mathcal{H}]$ are summarized as

$$\begin{aligned}
{}^{(2)}\mathcal{G}_{\eta}{}^{\eta} = \frac{2}{a^2}\Bigg[& -3D_k \stackrel{(1)}{\Phi} D^k \stackrel{(1)}{\Phi} - 8 \stackrel{(1)}{\Phi} \Delta \stackrel{(1)}{\Phi} - 3\left(\partial_\eta \stackrel{(1)}{\Phi}\right)^2 - 12\left(\mathcal{H}^2 + K\right)\left(\stackrel{(1)}{\Phi}\right)^2 + D_l D_k \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}{}^{lk} \\
& + \frac{1}{8}\partial_\eta \stackrel{(1)}{\chi}{}^{kl} \left(\partial_\eta + 8\mathcal{H}\right) \stackrel{(1)}{\chi}_{kl} + \frac{1}{2} D_k \stackrel{(1)}{\chi}_{lm} D^{[l} \stackrel{(1)}{\chi}{}^{k]m} - \frac{1}{8} D_k \stackrel{(1)}{\chi}_{lm} D^k \stackrel{(1)}{\chi}{}^{ml} - \frac{1}{2} \stackrel{(1)}{\chi}{}^{lm} \left(\Delta - K\right) \stackrel{(1)}{\chi}_{lm} \Bigg],
\end{aligned} \tag{6.10}$$

$${}^{(2)}\mathcal{G}_{\eta}{}^{i} = \frac{2}{a^2}\left[8 \stackrel{(1)}{\Phi} \partial_\eta D^i \stackrel{(1)}{\Phi} - D_j \stackrel{(1)}{\Phi} \partial_\eta \stackrel{(1)}{\chi}{}^{ji} - \left(\partial_\eta D_j \stackrel{(1)}{\Phi} + 2\mathcal{H} D_j \stackrel{(1)}{\Phi}\right) \stackrel{(1)}{\chi}{}^{ij} + \frac{1}{4}\partial_\eta \stackrel{(1)}{\chi}_{jk} D^i \stackrel{(1)}{\chi}{}^{kj} + \stackrel{(1)}{\chi}_{kl} \partial_\eta D^{[i} \stackrel{(1)}{\chi}{}^{k]l} \right], \tag{6.11}$$

$${}^{(2)}\mathcal{G}_{i}{}^{\eta} = \frac{2}{a^2}\left[8\mathcal{H} \stackrel{(1)}{\Phi} D_i \stackrel{(1)}{\Phi} - 2 D_i \stackrel{(1)}{\Phi} \partial_\eta \stackrel{(1)}{\Phi} + D^j \stackrel{(1)}{\Phi} \partial_\eta \stackrel{(1)}{\chi}_{ij} - \partial_\eta D^j \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}_{ij} - \frac{1}{4}\partial_\eta \stackrel{(1)}{\chi}{}^{kj} D_i \stackrel{(1)}{\chi}_{kj} + \stackrel{(1)}{\chi}{}^{kj} \partial_\eta D_{[j} \stackrel{(1)}{\chi}_{i]k} \right], \tag{6.12}$$

$$\begin{aligned}
{}^{(2)}\mathcal{G}_{i}{}^{j} = \frac{2}{a^2}\Bigg[& \left\{ -3D_k \stackrel{(1)}{\Phi} D^k \stackrel{(1)}{\Phi} - 4 \stackrel{(1)}{\Phi} \left(\Delta + K\right) \stackrel{(1)}{\Phi} - \partial_\eta \stackrel{(1)}{\Phi} \partial_\eta \stackrel{(1)}{\Phi} - 8\mathcal{H} \stackrel{(1)}{\Phi} \partial_\eta \stackrel{(1)}{\Phi} - 4\left(2\partial_\eta \mathcal{H} + \mathcal{H}^2\right)\left(\stackrel{(1)}{\Phi}\right)^2 \right\} \gamma_i{}^j \\
& + 2D_i \stackrel{(1)}{\Phi} D^j \stackrel{(1)}{\Phi} + 4 \stackrel{(1)}{\Phi} D_i D^j \stackrel{(1)}{\Phi} + \stackrel{(1)}{\chi}_{i}{}^{j} \left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta\right) \stackrel{(1)}{\Phi} + D_k \stackrel{(1)}{\Phi} \left(D_i \stackrel{(1)}{\chi}{}^{jk} + D^j \stackrel{(1)}{\chi}_{ik} \right) \\
& - 2D^k \stackrel{(1)}{\Phi} D_k \stackrel{(1)}{\chi}_{i}{}^{j} - 2 \stackrel{(1)}{\Phi} \left(\Delta - 2K\right) \stackrel{(1)}{\chi}_{i}{}^{j} - \Delta \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}_{i}{}^{j} + D_k D_i \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}{}^{jk} + D^m D^j \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}_{im} - D_l D_k \stackrel{(1)}{\Phi} \stackrel{(1)}{\chi}{}^{lk} \gamma_i{}^j \\
& - \frac{1}{2}\partial_\eta \stackrel{(1)}{\chi}_{ik} \partial_\eta \stackrel{(1)}{\chi}{}^{kj} + D_k \stackrel{(1)}{\chi}_{il} D^{[k} \stackrel{(1)}{\chi}{}^{l]j} + \frac{1}{4} D^j \stackrel{(1)}{\chi}_{lk} D_i \stackrel{(1)}{\chi}{}^{lk} + \frac{1}{2} \stackrel{(1)}{\chi}_{lm} D_i D^j \stackrel{(1)}{\chi}{}^{ml} - \frac{1}{2} \stackrel{(1)}{\chi}_{lm} D^l D_i \stackrel{(1)}{\chi}{}^{mj} \\
& - \frac{1}{2} \stackrel{(1)}{\chi}{}^{lm} D_l D^j \stackrel{(1)}{\chi}_{mi} + \frac{1}{2} \stackrel{(1)}{\chi}{}^{lm} D_m D_l \stackrel{(1)}{\chi}_{i}{}^{j} - \frac{1}{2} \stackrel{(1)}{\chi}{}^{jk} \left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta - \Delta + 2K\right) \stackrel{(1)}{\chi}_{ik} \\
& + \frac{1}{2}\Bigg\{ \frac{3}{4}\partial_\eta \stackrel{(1)}{\chi}_{lk} \partial_\eta \stackrel{(1)}{\chi}{}^{kl} + \stackrel{(1)}{\chi}_{kl} \left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta - \Delta + K\right) \stackrel{(1)}{\chi}{}^{lk} - \frac{1}{4} D_k \stackrel{(1)}{\chi}_{lm} D^k \stackrel{(1)}{\chi}{}^{ml} \\
& \qquad + D_k \stackrel{(1)}{\chi}_{lm} D^{[l} \stackrel{(1)}{\chi}{}^{k]m} \Bigg\} \gamma_i{}^j \Bigg].
\end{aligned} \tag{6.13}$$

We have checked the identity (3.14) through Eqs. (6.10)–(6.13), Then, we may say that the expressions (6.10)–

(6.13) are self-consistent.

C. Energy-momentum tensor and Klein-Gordon equation

Here, we summarize the explicit components of the gauge-invariant parts (3.23) of the second-order perturbation of energy momentum tensor for a single scalar field in terms of gauge-invariant variables. Through Eqs. (4.4), (5.4), (6.1), the components of Eq. (3.23) are derived by the straightforward calculations. In this paper, we just summarize the components of ${}^{(2)}\mathcal{T}_a^{\ b}$ in the situation where the first-order Einstein equations (5.12) and (5.16) are satisfied:

$$
\begin{aligned}
a^{2\,(2)}\mathcal{T}_\eta^{\ \eta} &= -\partial_\eta\varphi\partial_\eta\varphi_2 + (\partial_\eta\varphi)^2 \overset{(2)}{\Phi} - a^2\varphi_2\frac{\partial V}{\partial\varphi} + 4\partial_\eta\varphi \overset{(1)}{\Phi} \partial_\eta\varphi_1 - 4(\partial_\eta\varphi)^2\left(\overset{(1)}{\Phi}\right)^2 - (\partial_\eta\varphi_1)^2 \\
&\quad - D_i\varphi_1 D^i\varphi_1 - a^2(\varphi_1)^2\frac{\partial^2 V}{\partial\varphi^2}, \qquad (6.14) \\
a^{2\,(2)}\mathcal{T}_i^{\ \eta} &= -\partial_\eta\varphi D_i\varphi_2 + 4\partial_\eta\varphi D_i\varphi_1 \overset{(1)}{\Phi} - 2D_i\varphi_1\partial_\eta\varphi_1, \qquad (6.15) \\
a^{2\,(2)}\mathcal{T}_\eta^{\ i} &= \partial_\eta\varphi D^i\varphi_2 + 2\partial_\eta\varphi_1 D^i\varphi_1 + 4\partial_\eta\varphi \overset{(1)}{\Phi} D^i\varphi_1 - 2\partial_\eta\varphi \overset{(1)}{\chi}{}^{il} D_l\varphi_1, \qquad (6.16) \\
a^{2\,(2)}\mathcal{T}_i^{\ j} &= D_i\varphi_1 D^j\varphi_1 + \frac{1}{2}\gamma_i^{\ j}\left\{\partial_\eta\varphi\partial_\eta\varphi_2 - 4\partial_\eta\varphi \overset{(1)}{\Phi} \partial_\eta\varphi_1 + 4(\partial_\eta\varphi)^2\left(\overset{(1)}{\Phi}\right)^2 - (\partial_\eta\varphi)^2 \overset{(2)}{\Phi} + (\partial_\eta\varphi_1)^2\right. \\
&\qquad\qquad \left. - D_l\varphi_1 D^l\varphi_1 - a^2\varphi_2\frac{\partial V}{\partial\varphi} - a^2(\varphi_1)^2\frac{\partial^2 V}{\partial\varphi^2}\right\}. \qquad (6.17)
\end{aligned}
$$

More generic formulae for the components of ${}^{(2)}\mathcal{T}_a^{\ b}$ are given in Ref. [12].

Next, we show the gauge-invariant second-order the Klein-Gordon equation. We only consider the simple situation where Eqs. (5.12) and (5.16) are satisfied. The formulae for more generic situation is given in Ref. [12]. Through Eqs. (5.4), (6.1), (4.4), the second-order perturbation of the Klein-Gordon equation (3.29) is given by

$$
\begin{aligned}
-a^2 \overset{(2)}{\mathcal{C}}_{(K)} &= \partial_\eta^2\varphi_2 + 2\mathcal{H}\partial_\eta\varphi_2 - \Delta\varphi_2 \\
&\quad - \left(\partial_\eta \overset{(2)}{\Phi} + 3\partial_\eta \overset{(2)}{\Psi}\right)\partial_\eta\varphi \\
&\quad + 2a^2 \overset{(2)}{\Phi} \frac{\partial V}{\partial\bar{\varphi}}(\varphi) + a^2\varphi_2\frac{\partial^2 V}{\partial\bar{\varphi}^2}(\varphi) \\
&\quad - \Xi_{(K)} \\
&= 0, \qquad (6.18)
\end{aligned}
$$

where we defined

$$
\begin{aligned}
\Xi_{(K)} &:= 8\partial_\eta \overset{(1)}{\Phi} \partial_\eta\varphi_1 + 8 \overset{(1)}{\Phi} \Delta\varphi_1 - 4a^2 \overset{(1)}{\Phi} \varphi_1\frac{\partial^2 V}{\partial\bar{\varphi}^2}(\varphi) \\
&\quad - a^2(\varphi_1)^2\frac{\partial^3 V}{\partial\bar{\varphi}^3}(\varphi) + 8 \overset{(1)}{\Phi} \partial_\eta \overset{(1)}{\Phi} \partial_\eta\varphi \\
&\quad - 2 \overset{(1)}{\chi}{}^{ij} D_j D_i\varphi_1 + \partial_\eta\varphi \overset{(1)}{\chi}{}^{ij} \partial_\eta \overset{(1)}{\chi}_{ij}. \qquad (6.19)
\end{aligned}
$$

In Eq. (6.18), $\Xi_{(K)}$ is the source term which is the collection of the quadratic terms of the linear-order perturbations in the second-order perturbation of the Klein-Gordon equation. If we ignore this source term, Eq. (6.18) coincide with the first-order perturbation of the Klein-Gordon equation. From this source term (6.19) of the Klein-Gordon equation, we can see that the mode-mode coupling due to the non-linear effects appear in the second-order Klein-Gordon equation.

We cannot discuss solutions to Eq. (6.18) only through this equation, since this includes metric perturbations. To determine the behavior of the metric perturbations, we have to treat the Einstein equations simultaneously. The second-order Einstein equation is shown in Sec. VI D.

D. Einstein equations

Here, we show the all components of the second-order Einstein equation (3.33). All components of Eq. (3.33) are summarized as

$$
\begin{aligned}
&\left(-3\mathcal{H}\partial_\eta + \Delta + 3K\right) \overset{(2)}{\Psi} + \left(-\partial_\eta\mathcal{H} - 2\mathcal{H}^2 + K\right) \overset{(2)}{\Phi} \\
&\quad - 4\pi G\left(\partial_\eta\varphi\partial_\eta\varphi_2 + a^2\varphi_2\frac{\partial V}{\partial\varphi}\right) = \Gamma_0, \qquad (6.20)
\end{aligned}
$$

$$
\begin{aligned}
&2\partial_\eta D_i \overset{(2)}{\Psi} + 2\mathcal{H}D_i \overset{(2)}{\Phi} - \frac{1}{2}(\Delta + 2K) \overset{(2)}{\nu}_i \\
&\quad - 8\pi G D_i\varphi_2\partial_\eta\varphi = \Gamma_i, \qquad (6.21)
\end{aligned}
$$

$$
\begin{aligned}
&D_iD_j\left(\overset{(2)}{\Psi} - \overset{(2)}{\Phi}\right) + \left\{\left(-\Delta + 2\partial_\eta^2 + 4\mathcal{H}\partial_\eta - 2K\right)\overset{(2)}{\Psi} + \left(2\mathcal{H}\partial_\eta + 2\partial_\eta\mathcal{H} + 4\mathcal{H}^2 + \Delta + 2K\right)\overset{(2)}{\Phi}\right\}\gamma_{ij} \\
&-\frac{1}{a^2}\partial_\eta\left(a^2 D_{(i}\overset{(2)}{\nu}_{j)}\right) + \frac{1}{2}\left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta\right)\overset{(2)}{\chi}_{ij} - 8\pi G\left(\partial_\eta\varphi\partial_\eta\varphi_2 - a^2\varphi_2\frac{\partial V}{\partial\varphi}(\varphi)\right)\gamma_{ij} = \Gamma_{ij}, \qquad (6.22)
\end{aligned}
$$

where Γ_0, Γ_i Γ_{ij} are the collection of the quadratic term of the first-order perturbations as follows:

$$
\begin{aligned}
\Gamma_0 \;:=\; & 4\pi G\left((\partial_\eta\varphi_1)^2 + D_i\varphi_1 D^i\varphi_1 + a^2(\varphi_1)^2\frac{\partial^2 V}{\partial\varphi^2}\right) - 4\partial_\eta\mathcal{H}\left(\overset{(1)}{\Phi}\right)^2 - 2\overset{(1)}{\Phi}\partial_\eta^2\overset{(1)}{\Phi} - 3D_k\overset{(1)}{\Phi}D^k\overset{(1)}{\Phi} - 10\overset{(1)}{\Phi}\Delta\overset{(1)}{\Phi} \\
& -3\left(\partial_\eta\overset{(1)}{\Phi}\right)^2 - 16K\left(\overset{(1)}{\Phi}\right)^2 - 8\mathcal{H}^2\left(\overset{(1)}{\Phi}\right)^2 + D_lD_k\overset{(1)}{\Phi}\overset{(1)}{\chi}{}^{lk} + \frac{1}{8}\partial_\eta\overset{(1)}{\chi}_{lk}\partial_\eta\overset{(1)}{\chi}{}^{kl} + \mathcal{H}\overset{(1)}{\chi}_{kl}\partial_\eta\overset{(1)}{\chi}{}^{lk} \\
& -\frac{3}{8}D_k\overset{(1)}{\chi}_{lm}D^k\overset{(1)}{\chi}{}^{ml} + \frac{1}{4}D_k\overset{(1)}{\chi}_{lm}D^l\overset{(1)}{\chi}{}^{mk} - \frac{1}{2}\overset{(1)}{\chi}{}^{lm}\Delta\overset{(1)}{\chi}_{lm} + \frac{1}{2}K\overset{(1)}{\chi}_{lm}\overset{(1)}{\chi}{}^{lm}; \qquad (6.23) \\
\Gamma_i \;:=\; & 16\pi G\partial_\eta\varphi_1 D_i\varphi_1 - 4\partial_\eta\overset{(1)}{\Phi}D_i\overset{(1)}{\Phi} + 8\mathcal{H}\overset{(1)}{\Phi}D_i\overset{(1)}{\Phi} - 8\overset{(1)}{\Phi}\partial_\eta D_i\overset{(1)}{\Phi} + 2D^j\overset{(1)}{\Phi}\partial_\eta\overset{(1)}{\chi}_{ji} - 2\partial_\eta D^j\overset{(1)}{\Phi}\overset{(1)}{\chi}_{ij} \\
& -\frac{1}{2}\partial_\eta\overset{(1)}{\chi}_{jk}D_i\overset{(1)}{\chi}{}^{kj} - \overset{(1)}{\chi}_{kl}\partial_\eta D_i\overset{(1)}{\chi}{}^{lk} + \overset{(1)}{\chi}{}^{kl}\partial_\eta D_k\overset{(1)}{\chi}_{il}; \qquad (6.24) \\
\Gamma_{ij} \;:=\; & 16\pi G D_i\varphi_1 D_j\varphi_1 + 8\pi G\left\{(\partial_\eta\varphi_1)^2 - D_l\varphi_1 D^l\varphi_1 - a^2(\varphi_1)^2\frac{\partial^2 V}{\partial\varphi^2}\right\}\gamma_{ij} - 4D_i\overset{(1)}{\Phi}D_j\overset{(1)}{\Phi} - 8\overset{(1)}{\Phi}D_iD_j\overset{(1)}{\Phi} \\
& + \left(6D_k\overset{(1)}{\Phi}D^k\overset{(1)}{\Phi} + 4\overset{(1)}{\Phi}\Delta\overset{(1)}{\Phi} + 2\left(\partial_\eta\overset{(1)}{\Phi}\right)^2 + 8\partial_\eta\mathcal{H}\left(\overset{(1)}{\Phi}\right)^2 + 16\mathcal{H}^2\left(\overset{(1)}{\Phi}\right)^2 + 16\mathcal{H}\overset{(1)}{\Phi}\partial_\eta\overset{(1)}{\Phi} - 4\overset{(1)}{\Phi}\partial_\eta^2\overset{(1)}{\Phi}\right)\gamma_{ij} \\
& -4\mathcal{H}\partial_\eta\overset{(1)}{\Phi}\overset{(1)}{\chi}_{ij} - 2\partial_\eta^2\overset{(1)}{\Phi}\overset{(1)}{\chi}_{ij} - 4D^k\overset{(1)}{\Phi}D_{(i}\overset{(1)}{\chi}_{j)k} + 4D^k\overset{(1)}{\Phi}D_k\overset{(1)}{\chi}_{ij} - 8K\overset{(1)}{\Phi}\overset{(1)}{\chi}_{ij} + 4\overset{(1)}{\Phi}\Delta\overset{(1)}{\chi}_{ij} - 4D^kD_{(i}\overset{(1)}{\Phi}\overset{(1)}{\chi}_{j)k} \\
& +2\Delta\overset{(1)}{\Phi}\overset{(1)}{\chi}_{ij} + 2D_lD_k\overset{(1)}{\Phi}\overset{(1)}{\chi}{}^{lk}\gamma_{ij} + \partial_\eta\overset{(1)}{\chi}_{ik}\partial_\eta\overset{(1)}{\chi}_j{}^k - D^k\overset{(1)}{\chi}_{il}D_k\overset{(1)}{\chi}_j{}^l + D^k\overset{(1)}{\chi}_{il}D^l\overset{(1)}{\chi}_{jk} - \frac{1}{2}D_i\overset{(1)}{\chi}{}^{lk}D_j\overset{(1)}{\chi}_{lk} \\
& -\overset{(1)}{\chi}_{lm}D_iD_j\overset{(1)}{\chi}{}^{ml} + 2\overset{(1)}{\chi}{}^{lm}D_lD_{(i}\overset{(1)}{\chi}_{j)m} - \overset{(1)}{\chi}{}^{lm}D_mD_l\overset{(1)}{\chi}_{ij} \\
& -\frac{1}{4}\left(3\partial_\eta\overset{(1)}{\chi}_{lk}\partial_\eta\overset{(1)}{\chi}{}^{kl} - 3D_k\overset{(1)}{\chi}_{lm}D^k\overset{(1)}{\chi}{}^{ml} + 2D_k\overset{(1)}{\chi}_{lm}D^l\overset{(1)}{\chi}{}^{mk} - 4K\overset{(1)}{\chi}_{lm}\overset{(1)}{\chi}{}^{lm}\right)\gamma_{ij}. \qquad (6.25)
\end{aligned}
$$

Here, we used Eqs. (4.8), (5.12), (5.14), (5.16) and (5.18).

The tensor part of Eq. (6.22) is given by

$$
\begin{aligned}
\left(\partial_\eta^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta\right)\overset{(2)}{\chi}_{ij} \;=\; & 2\Gamma_{ij} - \frac{2}{3}\gamma_{ij}\Gamma_k{}^k - 3\left(D_iD_j - \frac{1}{3}\gamma_{ij}\Delta\right)(\Delta + 3K)^{-1}\left(\Delta^{-1}D^kD_l\Gamma_k{}^l - \frac{1}{3}\Gamma_k{}^k\right) \\
& +4\left\{D_{(i}(\Delta + 2K)^{-1}D_{j)}\Delta^{-1}D^lD_k\Gamma_l{}^k - D_{(i}(\Delta + 2K)^{-1}D^k\Gamma_{j)k}\right\}. \qquad (6.26)
\end{aligned}
$$

This tensor mode is also called the second-order gravitational waves.

Further, the vector part of Eqs. (6.21) and (6.22) yields the initial value constraint and the evolution equation of the vector mode $\overset{(2)}{\nu}_j$:

$$
\overset{(2)}{\nu}_i = \frac{2}{\Delta + 2K}\left\{D_i\Delta^{-1}D^k\Gamma_k - \Gamma_i\right\}, \quad \partial_\eta\left(a^2\overset{(2)}{\nu}_i\right) = \frac{2a^2}{\Delta + 2K}\left\{D_i\Delta^{-1}D^kD_l\Gamma_k{}^l - D_k\Gamma_i{}^k\right\}. \qquad (6.27)
$$

Finally, scalar part of Eqs. (6.21)–(6.22) are summarized as

$$2\partial_\eta \overset{(2)}{\Psi} + 2\mathcal{H} \overset{(2)}{\Phi} - 8\pi G \varphi_2 \partial_\eta \varphi = \Delta^{-1} D^k \Gamma_k, \tag{6.28}$$

$$\overset{(2)}{\Psi} - \overset{(2)}{\Phi} = \frac{3}{2}(\Delta + 3K)^{-1} \left\{ \Delta^{-1} D^i D_j \Gamma_i{}^j - \frac{1}{3}\Gamma_k{}^k \right\}, \tag{6.29}$$

$$\left(-\partial_\eta^2 - 5\mathcal{H}\partial_\eta + \frac{4}{3}\Delta + 4K\right) \overset{(2)}{\Psi} - \left(2\partial_\eta\mathcal{H} + \mathcal{H}\partial_\eta + 4\mathcal{H}^2 + \frac{1}{3}\Delta\right) \overset{(2)}{\Phi} - 8\pi G a^2 \varphi_2 \frac{\partial V}{\partial \varphi} = \Gamma_0 - \frac{1}{6}\Gamma_k{}^k, \tag{6.30}$$

$$\begin{aligned}
&\left\{ \partial_\eta^2 + 2\left(\mathcal{H} - \frac{\partial_\eta^2\varphi}{\partial_\eta\varphi}\right)\partial_\eta - \Delta - 4K + 2\left(\partial_\eta\mathcal{H} - \frac{\partial_\eta^2\varphi}{\partial_\eta\varphi}\mathcal{H}\right)\right\} \overset{(2)}{\Phi} \\
&\qquad = -\Gamma_0 - \frac{1}{2}\Gamma_k{}^k + \Delta^{-1} D^i D_j \Gamma_i{}^j + \left(\partial_\eta - \frac{\partial_\eta^2\varphi}{\partial_\eta\varphi}\right)\Delta^{-1} D^k \Gamma_k \\
&\qquad\quad - \frac{3}{2}\left\{ \partial_\eta^2 - \left(\frac{2\partial_\eta^2\varphi}{\partial_\eta\varphi} - \mathcal{H}\right)\partial_\eta \right\} (\Delta + 3K)^{-1} \left\{ \Delta^{-1} D^i D_j \Gamma_i{}^j - \frac{1}{3}\Gamma_k{}^k \right\}.
\end{aligned} \tag{6.31}$$

where $\Gamma_i{}^j := \gamma^{kj}\Gamma_{ik}$ and $\Gamma_k{}^k = \gamma^{ij}\Gamma_{ij}$. Eq. (6.31) is the second-order extension of Eq. (5.19), which is the master equation of scalar mode of the second-order cosmological perturbation in a universe filled with a single scalar field.

Thus, we have a set of ten equations for the second-order perturbations of a universe filled with a single scalar field, Eqs. (6.26)–(6.31). To solve this system of equations of the second-order Einstein equation, first of all, we have to solve the linear-order system. This is accomplished by solving Eq. (5.19) to obtain the potential $\overset{(1)}{\Phi}$, φ_1 is given through (5.14), and the tensor mode $\overset{(1)}{\chi}_{ij}$ is given by solving Eq. (5.17). Next, we evaluate the quadratic terms, Γ_0, Γ_i and Γ_{ij} of the linear-order perturbations, which are defined by Eqs. (6.23)–(6.25). Then, using the information of Eqs. (6.23)–(6.25), we estimate the source term in Eq. (6.31). If we know the two independent solutions to the linear-order master equation (5.19), we can solve Eq. (6.31) through the method using the Green functions. After constructing the solution $\overset{(2)}{\Phi}$ to Eq. (6.31), we can obtain the second-order metric perturbation $\overset{(2)}{\Psi}$ through Eq. (6.29). Thus, we have obtained the second-order gauge invariant perturbation φ_2 of the scalar field through Eq. (6.28). Thus, the all scalar modes $\overset{(2)}{\Phi}$, $\overset{(2)}{\Psi}$, φ_2 are obtained. Equation (6.30) is then used to check the consistency of the second-order perturbation of the Klein Gordon equation (6.18) as in Sec. VI E.

For the vector-mode, $\overset{(1)}{\nu_i}$ of the first-order identically vanishes due to the momentum constraint (5.16) for the linear-order metric perturbations. On the other hand, in the second-order, we have evolution equation (6.27) of the vector mode $\overset{(2)}{\nu_i}$ with the initial value constraint. This evolution equation of the second-order vector mode should be consistent with the initial value constraint, which is confirmed in Sec. VI E. Equations (6.27) also imply that the second-order vector-mode perturbation may be generated by the mode couplings of the linear order perturbations. As the simple situations, the generation of the second-order vector mode due to the scalar-scalar mode coupling is discussed in Refs. [26].

The second-order tensor mode is also generated by the mode-coupling of the linear-order perturbations through the source term in Eq. (6.26). Note that Eq. (6.26) is almost same as Eq. (5.17) for the linear-order tensor mode, except for the existence of the source term in Eq. (6.26). If we know the solution to the linear-order Einstein equations (5.17) and (5.19), we can evaluate the source term in Eq. (6.26). Further, we can solve Eq. (6.26) through the Green function method. This leads the generation of the gravitational wave of the second order. Actually, in the simple situation where the first-order tensor mode neglected, the generation of the second-order gravitational waves discussed in some literature[27].

E. Consistency of equations for second-order perturbations

Now, we consider the consistency of the second-order perturbations of the Einstein equations (6.28)–(6.31) for the scalar modes, Eqs. (6.27) for vector mode, and the Klein-Gordon equation (6.18). The consistency check of these equations are necessary to guarantee that the derived equations are correct, since the second-order Einstein equations have complicated forms owing to the quadratic terms of the linear-order perturbations that arise from the nonlinear effects of the Einstein equations.

Since the first equation in Eqs. (6.27) is the initial value constraint for the vector mode $\overset{(2)}{\nu_i}$ and it should be consistent with the evolution equation, i.e., the second equation of Eqs. (6.27). these equations should be consistent with each other from the general arguments of the Einstein equation. Explicitly, these equations are consistent with

each other if the equation

$$\partial_\eta \Gamma_k + 2\mathcal{H}\Gamma_k - D^l \Gamma_{lk} = 0 \tag{6.32}$$

is satisfied. Actually, through the first-order perturbative Einstein equations (5.14), (5.19), (5.17), we can confirm the equation (6.32). This is a trivial result from a general viewpoint, because the Einstein equation is the first class constrained system. However, this trivial result implies that we have derived the source terms Γ_i and Γ_{ij} of the second-order Einstein equations consistently.

Next, we consider Eq. (6.30). Through the second-order Einstein equations (6.28), (6.29), (6.31), and the background Klein-Gordon equation (4.9), we can confirm that Eq. (6.30) is consistent with the set of the background, first-order and other second-order Einstein equation if the equation

$$(\partial_\eta + 2\mathcal{H})\, D^k \Gamma_k - D^j D^i \Gamma_{ij} = 0 \tag{6.33}$$

is satisfied under the background and first-order Einstein equations. Actually, we have already seen that Eq. (6.32) is satisfied under the background and first-order Einstein equations. Taking the divergence of Eq. (6.32), we can immediately confirm Eq. (6.33). Then, Eq. (6.30) gives no information.

Thus, we have seen that the derived Einstein equations of the second order (6.27)–(6.31) are consistent with each other through Eq. (6.32). This fact implies that the derived source terms Γ_i and Γ_{ij} of the second-order perturbations of the Einstein equations, which are defined by Eqs. (6.24) and (6.25), are correct source terms of the second-order Einstein equations. On the other hand, for Γ_0, we have to consider the consistency between the perturbative Einstein equations and the perturbative Klein-Gordon equation as seen below.

Now, we consider the consistency of the second-order perturbation of the Klein-Gordon equation and the Einstein equations. The second-order perturbation of the Klein-Gordon equation is given by Eq. (6.18) with the source term (6.19). Since the vector mode $\overset{(2)}{\nu}_i$ and tensor mode $\overset{(2)}{\chi}_{ij}$ of the second-order do not appear in the expressions (6.18) of the second-order perturbation of the Klein-Gordon equation, we may concentrate on the Einstein equations for scalar mode of the second order, i.e., Eqs. (6.28), (6.29), and (6.31) with the definitions (6.23)–(6.25) of the source terms. As in the linear case, the second-order perturbation of the Klein-Gordon equation should also be derived from the set of equations consisting of the second-order perturbations of the Einstein equations (6.28), (6.29), (6.31), the first-order perturbations of the Einstein equations (5.12), (5.14), (5.19), and the background Einstein equations (4.6) and (4.7). Actually, from these equation, we can show that the second-order perturbation of the Klein-Gordon equation is consistent with the background and the second-order Einstein equations if the equation

$$\begin{aligned} 2\,(\partial_\eta + \mathcal{H})\,\Gamma_0 - D^k\Gamma_k + \mathcal{H}{\Gamma_k}^k & \\ +8\pi G \partial_\eta \varphi \Xi_{(K)} = 0 & \end{aligned} \tag{6.34}$$

is satisfied under the background and the first-order Einstein equations. Further, we can also confirm Eq. (6.34) through the background Einstein equations (4.6) and (4.7), the scalar part of the first-order perturbation of the momentum constraint (5.14), the evolution equations (5.19) and (5.17) for the first order scalar and tensor modes in the Einstein equation.

As shown in Ref. [13], the first-order perturbation of the Klein-Gordon equation is derived from the background and the first-order perturbations of the Einstein equation. In the case of the second-order perturbation, the Klein-Gordon equation (6.18) can be also derived from the background, the first-order, and the second-order Einstein equations. The second-order perturbations of the Einstein equation and the Klein-Gordon equation include the source terms Γ_0, Γ_i, Γ_{ij}, and $\Xi_{(K)}$ due to the mode-coupling of the linear-order perturbations. The second-order perturbation of the Klein-Gordon equation gives the relation (6.34) between the source terms Γ_0, Γ_i, Γ_{ij}, $\Xi_{(K)}$ and we have also confirmed that Eq. (6.34) is satisfied due to the background, the first-order perturbation of the Einstein equations, and the Klein-Gordon equation. Thus, the second-order perturbation of the Klein-Gordon equation is not independent of the set of the background, the first-order, and the second-order Einstein equations if we impose on the Einstein equation at any conformal time η. This also implies that the derived formulae of the source terms Γ_0, Γ_i, Γ_{ij}, and $\Xi_{(K)}$ are consistent with each other. In this sense, we may say that the formulae (6.23)–(6.25) and (6.19) for these source terms are correct.

VII. SUMMARY AND DISCUSSIONS

In this paper, we summarized the current status of the formulation of the gauge-invariant second-order cosmological perturbations. Although the presentation in this paper is restricted to the case of the universe filled by a single scalar field, the essence of the general framework of the gauge-invariant perturbation theory is transparent through this simple case. The general framework of the general relativistic higher-order gauge-invariant perturbation theory can be separated into three parts. First one is the general formulation to derive the gauge-transformation rules (2.18) and (2.19). Second one is the construction of the gauge-invariant variables for the perturbations on the generic background spacetime inspecting gauge-transformation rules (2.18) and (2.19) and the decomposition formula (2.36) and (2.37) for perturbations of any tensor field. Third one is the application of the above general framework of the gauge-invariant perturbation theory to the cosmological situations.

To derive the gauge-transformation rules (2.18) and (2.19), we considered the general arguments on the Taylor expansion of an arbitrary tensor field on a manifold, the general class of the diffeomorphism which is wider than the usual exponential map, and the general for-

mulation of the perturbation theory. This general class of diffeomorphism is represented in terms of the Taylor expansion (2.2) of its pull-back. As commented in Sec. II A, this general class of diffeomorphism does not form a one-parameter group of diffeomorphism as shown through Eq. (2.3). However, the properties (2.3) do not directly mean that this general class of diffeomorphism does not form a group. One of the key points of the properties of this diffeomorphism is the non-commutativity of generators ξ_1^a and ξ_2^a of each order. Although the expression of the n-th order Taylor expansion of the pull-back of this general class is discussed in Ref. [22], when we consider the situation of the n-th order perturbation, this non-commutativity becomes important[8]. Therefore, to clarify the properties of this general class of diffeomorphism, we have to take care of this non-commutativity of generators. Thus, there is a room to clarify the properties of this general class of diffeomorphism.

Further, in Sec. II C, we introduced a gauge choice $\mathcal{X}_\lambda$ as an exponential map, for simplicity. On the other hand, we have the concept of the general class of diffeomorphism which is wider than the class of the exponential map. Therefore, we may introduce a gauge choice as one of the element of this general class of diffeomorphism. However, the gauge-transformation rules (2.18) and (2.19) will not be changed even if we generalize the definition of a each gauge choice as emphasized in Sec. II C. Although there is a room to sophisticate in logical arguments to derive the gauge-transformation rules (2.18) and (2.19), these are harmless to the development of the general framework of the gauge-invariant perturbation theory shown in Secs. II C, II E, III, and their application to cosmological perturbations in Sec. IV.

As emphasize in Sec. II E, our starting point to construct gauge invariant variables is the assumption that *we already know the procedure for finding gauge invariant variables for the linear metric perturbations as Eq. (2.23).* This is highly nontrivial assumption on a generic background spacetime. The procedure to accomplish the decomposition (2.23) completely depends on the details of the background spacetime. In spite of this non-triviality, this assumption is almost correct in some background spacetime[28]. Further, once we accept this assumption, we can develop the higher-order perturbation theory in an independent manner of the details of the background spacetime. We also expect that this general framework of the gauge-invariant perturbation theory is extensible to n-th order perturbation theory, since our procedure to construct gauge-invariant variables can be extended to the third-order perturbation theory with two-parameter[8]. Due to this situation, in Ref. [12], we propose the conjecture which state that the above assumption for the decomposition of the linear-order metric perturbation is correct for any background spacetime. We may also say that the most nontrivial part of our general framework of higher-order gauge-invariant perturbation theory is in the above assumption. Further, as emphasized in Sec. V A, we assumed the existence of some Green functions to accomplish the decomposition (2.23) and this assumption exclude some perturbative modes of the metric perturbations from our consideration, even in the case of cosmological perturbations. For example, homogeneous modes of perturbations are excluded in our current arguments of the cosmological perturbation theory. These homogeneous modes will be necessary to discuss the comparison with the arguments based on the long-wavelength approximation. Therefore, we have to say that there is a room to clarify even in the cosmological perturbation theory.

Even if the assumption is correct on any background spacetime, the other problem is in the interpretations of the gauge-invariant variables. We have commented on the non-uniqueness in the definitions of the gauge-invariant variables through Eqs. (5.5) and (6.5). This non-uniqueness in the definition of gauge-invariant variables also leads some ambiguities in the interpretations of gauge-invariant variables. On the other hand, as emphasize in Sec. II C, any observations and experiments are carried out only on the physical spacetime through the physical processes on the physical spacetime. For this reason, any direct observables in any observations and experiments should be independent of the gauge choice. Further, the non-uniqueness in the definitions the gauge-invariant variables expressed by Eqs. (5.5) and (6.5) have the same form as the decomposition formulae (2.36) and (2.37). Therefore, if the statement that *any direct observables in any observations and experiments is independent of the gauge choice* is really true, this also confirm that the non-uniqueness of the definition of the gauge-invariant variables also have nothing to do with the direct observables in observations and experiments. These will be confirmed by the clarification of the relations between gauge-invariant variables and observables in experiments and observations. To accomplish this, we have to specify the concrete process of experiments and observations and clarify the problem what are the direct observables in the experiments and observations and derive the relations between the gauge-invariant variables and observables in concrete observations and experiments. If these arguments are completed, we will be able to show that the gauge degree of freedom is just unphysical degree of freedom and the non-uniqueness of the gauge-invariant variables have nothing to do with the direct observables in the concrete observation or experiment, and then, we will be able to clarify the precise physical interpretation of the gauge-invariant variables.

For example, in the case of the CMB physics, we can easily see that the first-order perturbation of the CMB temperature is automatically gauge invariant from Eq. (2.36), because the background temperature of CMB is homogeneous. On the other hand, the decomposition formula (2.37) of the second order yields that the theoretical prediction of the second-order perturbation of the CMB temperature may depend on gauge choice, since we do know the existence of the first-order fluctuations as the temperature anisotropy in CMB. However,

as emphasized above, the direct observables in observations should be gauge invariant and the gauge-variant term in Eq. (2.37) should be disappear in the direct observables. Therefore, we have to clarify the how gauge-invariant variables are related to the observed temperature fluctuations and the gauge-variant term disappear in the observable.

Although there are some rooms to accomplish the complete formulation of the second-order cosmological perturbation theory, we derived all the components of the second-order perturbation of the Einstein equation without ignoring any types modes (scalar-, vector-, tensor-types) of perturbations in the case of a scalar field system. In our formulation, any gauge fixing is not necessary and we can obtain all equations in the gauge-invariant form, which are equivalent to the complete gauge fixing. In other words, our formulation gives complete gauge-fixed equations without any gauge fixing. Therefore, equations obtained in a gauge-invariant manner cannot be reduced without physical restrictions any more. In this sense, the equations shown here are irreducible. This is one of the advantages of the gauge-invariant perturbation theory.

The resulting Einstein equations of the second order show that any type of mode-coupling appears as the quadratic terms of the linear-order perturbations owing to the nonlinear effect of the Einstein equations, in principle. Perturbations in cosmological situations are classified into three types: scalar, vector, and tensor. In the second-order perturbations, we also have these three types of perturbations as in the case of the first-order perturbations. Furthermore, in the equations for the second-order perturbations, there are many quadratic terms of linear-order perturbations owing to the nonlinear effects of the system. Owing to these nonlinear effects, the above three types of perturbations couple with each other. In the scalar field system shown in this paper, the first-order vector mode does not appear due to the momentum constraint of the first-order perturbation of the Einstein equation. Therefore, we have seen that three types of mode-coupling appear in the second-order Einstein equations, i.e., scalar-scalar, scalar-tensor, and tensor-tensor type of mode coupling. In general, all types of mode-coupling may appear in the second-order Einstein equations. Actually, in Ref. [13], we also derived the all components of the Einstein equations for a perfect fluid system and we can see all types of mode-coupling, i.e., scalar-scalar, scalar-vector, scalar-tensor, vector-vector, vector-tensor, tensor-tensor types mode-coupling, appear in the second-order Einstein equation, in general. Of course, in the some realistic situations of cosmology, we may neglect some modes. In this case, we may neglect some mode-coupling. However, even in this case, we should keep in mind the fact that all types of mode-couplings may appear in principle when we discuss the realistic situations of cosmology. We cannot deny the possibility that the mode-couplings of any type produces observable effects when the quite high accuracy of observations is accomplished.

Even in the case of the single scalar field discussed in this paper, the source terms of the second-order Einstein equation show the mode-coupling of scalar-scalar, scalar-tensor, and the tensor-tensor types as mentioned above. Since the tensor mode of the linear order is also generated due to quantum fluctuations during the inflationary phase, the mode-couplings of the scalar-tensor and tensor-tensor types may appear in the inflation. If these mode-couplings occur during the inflationary phase, these effects will depend on the scalar-tensor ratio r. If so, there is a possibility that the accurate observations of the second-order effects in the fluctuations of the scalar type in our universe also restrict the scalar-tensor ratio r or give some consistency relations between the other observations such as the measurements of the B-mode of the polarization of CMB. This will be a new effect that gives some information on the scalar-tensor ratio r.

Furthermore, we have also checked the consistency between the second-order perturbations of the equations of motion of matter field and the Einstein equations. In the case of a scalar field, we checked the consistency between the second-order perturbations of the Klein-Gordon equation and the Einstein equations. Due to this consistency check, we have obtained the consistency relations between the source terms in these equations Γ_0, Γ_i, Γ_{ij}, and $\Xi_{(K)}$, which are given by Eqs. (6.32) and (6.34). We note that the relation (6.32) comes from the consistency in the Einstein equations of the second order by itself, while the relation (6.34) comes from the consistency between the second-order perturbation of the Klein-Gordon equation and the Einstein equation. We also showed that these relations between the source terms are satisfied through the background and the first-order perturbation of the Einstein equations in Ref. [13]. This implies that the set of all equations are self-consistent and the derived source terms Γ_0, Γ_i, Γ_{ij}, and $\Xi_{(K)}$ are correct. We also note that these relations are independent of the details of the potential of the scalar field.

Thus, we have derived the self-consistent set of equations of the second-order perturbation of the Einstein equations and the evolution equations of matter fields in terms of gauge-invariant variables. As the current status of the second-order gauge-invariant cosmological perturbation theory, we may say that the curvature terms in the second-order Einstein tensor (3.33), i.e., the second-order perturbations of the Einstein tensor, are almost completely derived although there remains the problem of homogeneous modes as mentioned above. After complete the problem of homogeneous modes, we have to clarify the physical behaviors of the second-order cosmological perturbation in the single scalar field system in the context of the inflationary scenario. This is the preliminary step to clarify the quantum behaviors of second-order perturbations in the inflationary universe. Further, we also have to carry out the comparison with the result by long-wavelength approximations. If these issues are completed, we may say that we have completely un-

derstood the properties of the second-order perturbation of the Einstein tensor. The next task is to clarify the nature of the second-order perturbation of the energy-momentum tensor through the extension to multi-fluid or multi-field systems. Further, we also have to extend our arguments to the Einstein Boltzmann system to discuss CMB physics, since we have to treat photon and neutrinos through the Boltzmann distribution functions. This issue is also discussed in some literature[7, 14]. If we accomplish these extension, we will be able to clarify the Non-linear effects in CMB physics.

Finally, readers might think that the ingredients of this paper is too mathematical as Astronomy. However, we have to emphasize that a high degree of the theoretical sophistication leads unambiguous theoretical predictions in many case. As in the case of the linear-order cosmological perturbation theory, the developments in observations are also supported by the theoretical sophistication and the theoretical sophistication are accomplished motivated by observations. In this sense, now, we have an opportunity to develop the general relativistic second-order perturbation theory to a high degree of sophistication which is motivated by observations. We also expect that this theoretical sophistication will be also useful to discuss the theoretical predictions of Non-Gaussianity in CMB and comparison with observations. Therefore, I think that this opportunity is opened not only for observational cosmologists but also for theoretical and mathematical physicists.

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Appendix A: Derivation of the generic representation of the Taylor expansion of tensors on a manifold

In this section, we derive the representation of the coefficients of the formal Taylor expansion (2.2) of the pull-back of a diffeomorphism in terms of the suitable derivative operators. The guide principle of our arguments is the following theorem[20, 23].

Theorem A.1. *Let $\mathcal{D}$ be a derivative operator acting on the set of all the tensor fields defined on a differentiable manifold $\mathcal{M}$ and satisfying the following conditions: (i) it is linear and satisfies the Leibniz rule; (ii) it is tensor-type preserving; (iii) it commutes with every contraction of a tensor field; and (iv) it commutes with the exterior differentiation d. Then, $\mathcal{D}$ is equivalent to the Lie derivative operator with respect to some vector field ξ, i.e., $\mathcal{D} = \pounds_\xi$.*

The prove of the assertion of Theorem A.1 is given in Ref. [20] as follows. When acting on functions, the derivative operator $\mathcal{D}$ defines a vector field ξ through the relation

$$\mathcal{D}f =: \xi(f) = \pounds_\xi f, \quad \forall f \in \mathcal{F}(M). \tag{A1}$$

The assertion of the Theorem for an arbitrary tensor field is hold iff the assertions for an arbitrary scalar function and for an arbitrary vector field V are hold. To do this, we consider the scalar function $V(f)$ and we obtain

$$\mathcal{D}(V(f)) = \xi(V(f)) \tag{A2}$$

through Eq. (A1). Through the conditions (i)-(iv) of $\mathcal{D}$, $\mathcal{D}(V(f))$ is also given by

$$\begin{aligned}\mathcal{D}(V(f)) &= \mathcal{D}(df(V)) = \mathcal{D}\left\{\mathcal{C}(df\otimes V)\right\}\\ &= \mathcal{C}\left\{\mathcal{D}(df\otimes V)\right\}\\ &= \mathcal{C}\left\{\mathcal{D}(df)\otimes V + df\otimes\mathcal{D}V\right\}\\ &= \mathcal{C}\left\{d(\mathcal{D}f)\otimes V + df\otimes\mathcal{D}V\right\}\\ &= d(\mathcal{D}f)(V) + df(\mathcal{D}V)\\ &= V(\mathcal{D}f) + (\mathcal{D}V)(f)\end{aligned} \tag{A3}$$

Then we obtain

$$\begin{aligned}(\mathcal{D}V)(f) &= \xi(V(f)) - V(\xi(f)) = [\xi, V](f)\\ &= (\pounds_\xi V)(f)\end{aligned} \tag{A4}$$

for an arbitrary f, i.e.,

$$\mathcal{D}V = \pounds_\xi V. \tag{A5}$$

Through Eqs. (A1) and (A5), we can recursively show

$$\mathcal{D}Q = \pounds_\xi Q \tag{A6}$$

for an arbitrary tensor field Q[23].

Now, we consider the derivation of the Taylor expansion (2.1). As in the main text, we first consider the representation of the Taylor expansion of $\Phi^*_\lambda f$ for an arbitrary scalar function $f \in \mathcal{F}(M)$:

$$\begin{aligned}(\Phi^*_\lambda f)(p) &= f(p) + \lambda\left\{\frac{\partial}{\partial\lambda}(\Phi^*_\lambda f)\right\}_{\lambda=0}\\ &\quad +\frac{1}{2}\lambda^2\left\{\frac{\partial^2}{\partial\lambda^2}(\Phi^*_\lambda f)\right\}_{\lambda=0} + O(\lambda^3),\end{aligned} \tag{A7}$$

where $\mathcal{F}(M)$ denotes the algebra of C^∞ functions on $\mathcal{M}$. Although the operator $\partial/\partial\lambda$ in the bracket $\{*\}_{\lambda=0}$ of Eq. (A7) are simply symbolic notation, we stipulate the properties

$$\left\{\frac{\partial^2}{\partial\lambda^2}(\Phi^*_\lambda f)\right\}_{\lambda=0} = \left\{\frac{\partial}{\partial\lambda}\left(\frac{\partial}{\partial\lambda}(\Phi^*_\lambda f)\right)\right\}_{\lambda=0}, \tag{A8}$$

$$\left\{\frac{\partial}{\partial\lambda}(\Phi^*_\lambda f)^2\right\}_{\lambda=0} = \left\{2\Phi^*_\lambda f\frac{\partial}{\partial\lambda}(\Phi^*_\lambda f)\right\}_{\lambda=0}. \tag{A9}$$

for $\forall f \in \mathcal{F}(\mathcal{M})$, where n is an arbitrary finite integer. These properties imply that the operator $\partial/\partial\lambda$ is in fact not simply symbolic notation but indeed the usual partial differential operator on $\mathbb{R}$. We note that the property (A9) is the Leibniz rule, which plays important roles when we derive the representation of the Taylor expansion (A7) in terms of suitable Lie derivatives.

Together with the property (A9), Theorem A.1 yields that there exists a vector field ξ_1 so that

$$\left\{\frac{\partial}{\partial\lambda}(\Phi_\lambda^* f)\right\}_{\lambda=0} =: \pounds_{\xi_1} f. \tag{A10}$$

Actually, the conditions (ii)-(iv) in Theorem A.1 are satisfied from the fact that Φ_λ^* is the pull-back of a diffeomorphism Φ_λ and (i) is satisfied due to the property (A9).

Next, we consider the second-order term in Eq. (A7). Since we easily expect that the second-order term in Eq. (A7) may includes $\pounds_{\xi_1}^2$, we define the derivative operator $\mathcal{L}_2$ by

$$\left\{\frac{\partial^2}{\partial\lambda^2}(\Phi_\lambda^* f)\right\}_{\lambda=0} =: \left(\mathcal{L}_{(2)} + a\pounds_{\xi_1}^2\right) f, \tag{A11}$$

where a is determined so that $\mathcal{L}_2$ satisfy the conditions of Theorem A.1. The conditions (ii)-(iv) in Theorem A.1 for $\mathcal{L}_2$ are satisfied from the fact that Φ_λ^* is the pull-back of a diffeomorphism Φ_λ. Further, $\mathcal{L}_2$ is obviously linear but we have to check $\mathcal{L}_2$ satisfy the Leibniz rule, i.e.,

$$\mathcal{L}_2\left(f^2\right) = 2f\mathcal{L}_2 f \tag{A12}$$

for $\forall f \in \mathcal{F}(\mathcal{M})$. To do this, we use the properties (A8) and (A9), then we can easily see that the Leibniz rule (A12) is satisfied iff $a = 1$ and we may regard $\mathcal{L}_2$ as the Lie derivative with respect to some vector field. Then, when and only when $a = 1$, there exists a vector field ξ_2 such that

$$\mathcal{L}_2 f = \pounds_{\xi_2} f \tag{A13}$$

and

$$\left\{\frac{\partial^2}{\partial\lambda^2}(\Phi_\lambda^* f)\right\}_{\lambda=0} =: \left(\pounds_{\xi_2} + \pounds_{\xi_1}^2\right) f. \tag{A14}$$

Thus, we have seen that the Taylor expansion (A7) for an arbitrary scalar function f is given by Eq. (2.2).

Although the formula (2.2) of the Taylor expansion is for an arbitrary scalar function, we can easily extend this formula to that for an arbitrary tensor field Q as the assertion of Theorem A.1. The proof of the extension of the formula (2.2) to an arbitrary tensor field Q is completely parallel to the proof of the formula (2.2) for an arbitrary scalar function if we stipulate the properties

$$\left\{\frac{\partial^2}{\partial\lambda^2}(\Phi_\lambda^* Q)\right\}_{\lambda=0} = \left\{\frac{\partial}{\partial\lambda}\left(\frac{\partial}{\partial\lambda}(\Phi_\lambda^* Q)\right)\right\}_{\lambda=0}, \tag{A15}$$

$$\left\{\frac{\partial}{\partial\lambda}(\Phi_\lambda^* Q)^2\right\}_{\lambda=0} = \left\{2\Phi_\lambda^* Q\frac{\partial}{\partial\lambda}(\Phi_\lambda^* Q)\right\}_{\lambda=0} \tag{A16}$$

instead of Eqs. (A8) and (A9). As the result, we obtain the representation of the Taylor expansion for an arbitrary tensor field Q.

Appendix B: Derivation of the perturbative Einstein tensors

Following the outline of the calculations explained in Sec. III A, we first calculate the perturbative expansion of the inverse metric. The perturbative expansion of the inverse metric can be easily derived from Eq. (2.22) and the definition of the inverse metric

$$\bar{g}^{ab}\bar{g}_{bc} = \delta_c^a. \tag{B1}$$

We also expand the inverse metric $\bar{g}^{ab}$ in the form

$$\bar{g}^{ab} = g^{ab} + \lambda^{(1)}\bar{g}^{ab} + \frac{1}{2}\lambda^{2(2)}\bar{g}^{ab}. \tag{B2}$$

Then, each term of the expansion of the inverse metric is given by

$${}^{(1)}\bar{g}^{ab} = -h^{ab}, \quad {}^{(2)}\bar{g}^{ab} = 2h^{ac}h_c^{\ b} - l^{ab}. \tag{B3}$$

To derive the formulae for the perturbative expansion of the Riemann curvature, we have to derive the formulae for the perturbative expansion of the tensor $C^c_{\ ab}$ given by Eq. (3.3). The tensor $C^c_{\ ab}$ is also expanded in the same form as Eq. (2.11). The first-order perturbations of $C^c_{\ ab}$ have the well-known form[24]

$${}^{(1)}C^c_{\ ab} = \nabla_{(a}h_{b)}^{\ \ c} - \frac{1}{2}\nabla^c h_{ab} =: H_{ab}^{\ \ c}[h], \tag{B4}$$

where $H_{ab}^{\ \ c}[A]$ is defined by Eq. (3.11) for an arbitrary tensor field A_{ab} defined on the background spacetime $\mathcal{M}_0$. In terms of the tensor field $H_{ab}^{\ \ c}$ defined by (3.11) the second-order perturbation ${}^{(2)}C^c_{\ ab}$ of the tensor field $C^c_{\ ab}$ is given by

$${}^{(2)}C^c_{\ ab} = H_{ab}^{\ \ c}[l] - 2h^{cd}H_{abd}[h]. \tag{B5}$$

The Riemann curvature (3.4) on the physical spacetime $\mathcal{M}_\lambda$ is also expanded in the form (2.11):

$$\begin{aligned}\bar{R}_{abc}^{\ \ \ d} =: &\ R_{abc}^{\ \ \ d} + \lambda^{(1)}R_{abc}^{\ \ \ d} + +\frac{1}{2}\lambda^{2(2)}R_{abc}^{\ \ \ d} \\ &+O(\lambda^3).\end{aligned} \tag{B6}$$

The first- and the second-order perturbation of the Riemann curvature are given by

$${}^{(1)}R_{abc}^{\ \ \ d} = -2\nabla_{[a}{}^{(1)}C^d_{\ b]c}, \tag{B7}$$

$${}^{(2)}R_{abc}^{\ \ \ d} = -2\nabla_{[a}{}^{(2)}C^d_{\ b]c} + 4{}^{(1)}C^e_{\ c[a}{}^{(1)}C^d_{\ b]e} \tag{B8}$$

Substituting Eqs. (B4) and (B5) into Eqs. (B7) and (B8), we obtain the perturbative form of the Riemann curvature in terms of the variables defined by Eq. (3.11) and

(3.12):

$$
\begin{aligned}
{}^{(1)}R_{abc}{}^{d} &= -2\nabla_{[a}H_{b]c}{}^{d}[h], && \text{(B9)}\\
{}^{(2)}R_{abc}{}^{d} &= -2\nabla_{[a}H_{b]c}{}^{d}[l] + 4H_{[a}{}^{de}[h]\,H_{b]ce}[h]\\
&\quad +4h^{de}\nabla_{[a}H_{b]ce}[h]. && \text{(B10)}
\end{aligned}
$$

To write down the perturbative curvatures (B9) and (B10) in terms of the gauge invariant and variant variables defined by Eqs. (2.23) and (2.32), we first derive an expression for the tensor field $H_{abc}[h]$ in terms of the gauge invariant variables, and then, we derive a perturbative expression for the Riemann curvature.

First, we consider the linear-order perturbation (B9) of the Riemann curvature. Using the decomposition (2.23) and the identity $R_{[abc]}{}^{d} = 0$, we can easily derive the relation

$$
H_{abc}[h] = H_{abc}[\mathcal{H}] + \nabla_a\nabla_b X_c + R_{bca}{}^{d}X_d, \quad \text{(B11)}
$$

where the variable $H_{abc}[\mathcal{H}]$ is defined by Eqs. (3.11) and (3.12) with $A_{ab} = \mathcal{H}_{ab}$. Clearly, the variable $H_{ab}{}^{c}[\mathcal{H}]$ is gauge invariant. Taking the derivative and using the Bianchi identity $\nabla_{[a}R_{bc]de} = 0$, we obtain

$$
{}^{(1)}R_{abc}{}^{d} = -2\nabla_{[a}H_{b]c}{}^{d}[\mathcal{H}] + \pounds_X R_{abc}{}^{d}. \quad \text{(B12)}
$$

Similar but some cumbersome calculations yield

$$
\begin{aligned}
{}^{(2)}R_{abc}{}^{d} =& -2\nabla_{[a}H_{b]c}{}^{d}[\mathcal{L}] + 4H_{[a}{}^{de}[\mathcal{H}]\,H_{b]ce}[\mathcal{H}]\\
&+4\mathcal{H}_{e}{}^{d}\nabla_{[a}H_{b]c}{}^{e}[\mathcal{H}]\\
&+2\pounds_X {}^{(1)}R_{abc}{}^{d} + \left(\pounds_Y - \pounds_X^2\right)R_{abc}{}^{d}. \quad \text{(B13)}
\end{aligned}
$$

Equations (B12) and (B13) have the same for as the decomposition formulae (2.36) and (2.37), respectively.

Contracting the indices b and d in Eqs. (B12) and (B13) of the perturbative Riemann curvature, we can directly derive the formulae for the perturbative expansion of the Ricci curvature: expanding the Ricci curvature

$$
\bar{R}_{ab} =: R_{ab} + \lambda^{(1)}R_{ab} + +\frac{1}{2}\lambda^{2\,(2)}R_{ab} + O(\lambda^3), \quad \text{(B14)}
$$

we obtain the first-order Ricci curvature as

$$
{}^{(1)}R_{ab} = -2\nabla_{[a}H_{c]b}{}^{c}[\mathcal{H}] + \pounds_X R_{ab}. \quad \text{(B15)}
$$

and we also obtain the second-order Ricci curvature as

$$
\begin{aligned}
{}^{(2)}R_{ab} =& -2\nabla_{[a}H_{c]b}{}^{c}[\mathcal{L}] + 4H_{[a}{}^{cd}[\mathcal{H}]\,H_{c]bd}[\mathcal{H}]\\
&+4\mathcal{H}_{d}{}^{c}\nabla_{[a}H_{b]c}{}^{d}[\mathcal{H}]\\
&+2\pounds_X {}^{(1)}R_{ab} + \left(\pounds_Y - \pounds_X^2\right)R_{ab}. \quad \text{(B16)}
\end{aligned}
$$

The scalar curvature on the physical spacetime $\mathcal{M}$ is given by $\bar{R} = \bar{g}^{ab}\bar{R}_{ab}$. To obtain the perturbative form of the scalar curvature, we expand the $\bar{R}$ in the form (2.11), i.e.,

$$
\bar{R} =: R + \lambda^{(1)}R + \frac{1}{2}\lambda^{2\,(2)}R + O(\lambda^3) \quad \text{(B17)}
$$

and $\bar{g}^{ab}\bar{R}_{ab}$ is expanded through the Leibniz rule. Then, the perturbative formula for the scalar curvature at each order is derived from perturbative form of the inverse metric (B3) and the Ricci curvature (B15) and (B16). Straightforward calculations lead to the expansion of the scalar curvature as

$$
\begin{aligned}
{}^{(1)}R =& -2\nabla_{[a}H_{b]}{}^{ab}[\mathcal{H}] - R_{ab}\mathcal{H}^{ab} + \pounds_X R, && \text{(B18)}\\
{}^{(2)}R =& -2\nabla_{[a}H_{b]}{}^{ab}[\mathcal{L}] + R^{ab}\left(2\mathcal{H}_{ca}\mathcal{H}_{b}{}^{c} - \mathcal{L}_{ab}\right)\\
&+4H_{[a}{}^{cd}[\mathcal{H}]\,H_{c]}{}^{a}{}_{d}[\mathcal{H}] + 4\mathcal{H}_{c}{}^{b}\nabla_{[a}H_{b]}{}^{ac}[\mathcal{H}]\\
&+4\mathcal{H}^{ab}\nabla_{[a}H_{d]b}{}^{d}[\mathcal{H}]\\
&+2\pounds_X {}^{(1)}R + \left(\pounds_Y - \pounds_X^2\right)R. && \text{(B19)}
\end{aligned}
$$

We also note that the expansion formulae (B18) and (B19) have the same for as the decomposition formulae (2.36) and (2.37), respectively.

Next, we consider the perturbative form of the Einstein tensor $\bar{G}_{ab} := \bar{R}_{ab} - \frac{1}{2}\bar{g}_{ab}\bar{R}$ and we expand $\bar{G}_{ab}$ as in the form (2.11):

$$
\bar{G}_{ab} =: G_{ab} + \lambda^{(1)}(G_{ab}) + \frac{1}{2}\lambda^{2\,(2)}(G_{ab}) + O(\lambda^3). \quad \text{(B20)}
$$

As in the case of the scalar curvature, straightforward calculations lead

$$
\begin{aligned}
{}^{(1)}(G_{ab}) =& -2\nabla_{[a}H_{d]b}{}^{d}[\mathcal{H}] + g_{ab}\nabla_{[c}H_{d]}{}^{cd}[\mathcal{H}] - \frac{1}{2}R\mathcal{H}_{ab} + \frac{1}{2}g_{ab}R_{cd}\mathcal{H}^{cd} + \pounds_X G_{ab}, && \text{(B21)}\\
{}^{(2)}(G_{ab}) =& -2\nabla_{[a}H_{c]b}{}^{c}[\mathcal{L}] + 4H_{[a}{}^{cd}[\mathcal{H}]\,H_{c]bd}[\mathcal{H}] + 4\mathcal{H}_{c}{}^{d}\nabla_{[a}H_{d]b}{}^{c}[\mathcal{H}]\\
&-\frac{1}{2}g_{ab}\Big(-2\nabla_{[c}H_{d]}{}^{cd}[\mathcal{L}] + 2R_{de}\mathcal{H}_{c}{}^{d}\mathcal{H}^{ec} - R_{de}\mathcal{L}^{de} + 4H_{[c}{}^{de}[\mathcal{H}]\,H_{d]}{}^{c}{}_{e}[\mathcal{H}]\\
&\qquad +4\mathcal{H}_{e}{}^{d}\nabla_{[c}H_{d]}{}^{ce}[\mathcal{H}] + 4\mathcal{H}^{ce}\nabla_{[c}H_{d]e}{}^{d}[\mathcal{H}]\Big) + 2\mathcal{H}_{ab}\nabla_{[c}H_{d]}{}^{cd}[\mathcal{H}] + \mathcal{H}_{ab}\mathcal{H}^{cd}R_{cd} - \frac{1}{2}R\mathcal{L}_{ab}\\
&+2\pounds_X {}^{(1)}(G_{ab}) + \left(\pounds_Y - \pounds_X^2\right)G_{ab}. && \text{(B22)}
\end{aligned}
$$

We note again that Eqs. (B21) and (B22) have the same form as the decomposition formulae (2.36) and (2.37), respectively.

The perturbative formulae for the perturbation of the Einstein tensor

$$\bar{G}_a{}^b = \bar{g}^{bc}\bar{G}_{ac} \tag{B23}$$

is derived by the similar manner to the case of the perturbations of the scalar curvature. Through these formulae summarized above, straightforward calculations leads Eqs. (3.6)–(3.10). We have to note that to derive the formulae (3.9) with Eq. (3.10), we have to consider the general relativistic gauge-invariant perturbation theory with two infinitesimal parameters which is developed in Refs. [8, 9], as commented in the main text.

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